

Microscopic chaos and transport in thermostated dynamical systems

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A fundamental challenge is to understand nonequilibrium statistical mechanics starting from microscopic chaos in the equations of motion of a many-particle system. In this review we summarize recent theoretical advances along these lines. Particularly, we are concerned with nonequilibrium situations created by external electric fields and by temperature or velocity gradients. These constraints pump energy into a system, hence there must be some thermal reservoir that prevents the system from heating up. About twenty years ago a *deterministic and time-reversible modeling* of such thermal reservoirs was proposed in form of Gaussian and Nosé-Hoover thermostats. This approach yielded simple relations between fundamental quantities of nonequilibrium statistical mechanics and of dynamical systems theory. The main theme of our review is to critically assess the universality of these results. As a vehicle of demonstration we employ the driven periodic Lorentz gas, which is a toy model for the classical dynamics of an electron in a metal under application of an electric field. Applying different types of thermal reservoirs to this system we compare the resulting nonequilibrium steady states with each other. Along the same lines we discuss an interacting many-particle system under shear and heat. Finally, we outline an unexpected relationship between deterministic thermostats and active Brownian particles modeling biophysical cell motility.

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I. INTRODUCTION AND OUTLINE

Statistical mechanics endeavours to understand the origin of the macroscopic properties of matter starting from the microscopic equations of motion of single atoms or molecules. This program traces back to the founders of statistical mechanics, Boltzmann, Maxwell and Gibbs, and for many-particle systems in thermal equilibrium it was pursued with remarkable success, as is demonstrated in many textbooks, see, e.g., Refs. [Rei65,Hua87]. However, in nonequilibrium situations, that is, for systems under constraints such as external fields or by imposing temperature or velocity gradients, statistical mechanical theories appear to be rather incomplete. We just mention that in contrast to the equilibrium case there is no generally accepted definition of a nonequilibrium entropy, and correspondingly yet there is no general agreement on nonequilibrium ensembles that might replace the equilibrium ones [Pen79,Eva90b,Ger99,Rue99b,Gal99].

Fresh input concerning these fundamental problems came from the side of dynamical systems theory, in particular by work of mathematicians like Sinai, Ruelle, Bowen and others over the past few decades. Indeed, *SRB measures*¹ appear to provide good candidates for taking over the role of the Gibbs ensemble in nonequilibrium [Gas98a,Dor99,Gal99,Rue99b,You02,Gal03]. Additionally, the advent of powerful computers made it possible to solve numerically the nonlinear equations of motion of many-particle systems and to investigate the interplay between microscopic chaos in the collisions of the single particles and transport properties on macroscopic scales in much more detail than it was possible to the times of the founders of statistical mechanics.

The stage for this review is set by two basic approaches that evolved over the past two decades trying to develop a concise picture of nonequilibrium statistical mechanics by employing methods of dynamical systems theory. In the following two sections we briefly summarize important features of these two directions of research. We then sketch how the present review is embedded into the existing literature, outline its contents and also say some words about the style in which it is written.

A. The Hamiltonian dynamical systems approach to nonequilibrium steady states

In recent work Gaspard, Nicolis and Dorfman studied nonequilibrium situations by imposing specific boundary conditions onto spatially extended chaotic *Hamiltonian* dynamical systems. A typical example are diffusion processes due to concentration gradients at the boundaries. By this approach the macroscopic transport properties of deterministic dynamical systems could be linked to the underlying microscopic chaos in the equations of motion of the single particles in two ways: The *escape rate approach* considers dynamical systems with absorbing boundaries [Gas90, Gas92b, Gas93, Gas95a, Dor95, Gas95b, Gas98a, Dor99]. Here the escape rate determined by a statistical physical transport equation such as, for example, the diffusion equation, is matched to the one resulting from solving the Liouville equation of the dynamical system. This procedure yields simple formulas linking transport coefficients to dynamical systems quantities, which are here the positive Lyapunov exponents and the Kolmogorov-Sinai entropy of the dynamical system, or respectively the fractal dimension of the associated repeller of the open system.

A second, conceptually related approach applies to closed systems with periodic boundary conditions and has been worked out for diffusion [Gil01, Gas01] and for reaction-diffusion [Cla02] in low-dimensional model systems. In this case the decay rate to thermal equilibrium as obtained from the diffusion equation is related to the fractal dimension of the corresponding hydrodynamic mode in the Liouville equation of the dynamical system. The diffusion coefficient can thus be expressed as a function of the system's largest Lyapunov exponent combined with the Hausdorff dimension of this mode. Both approaches can consistently be derived by using Ruelle's thermodynamic formalism [Gas95b, Gas01]. A further interesting result obtained in this framework deals with the parameter dependence of transport coefficients. By employing that statistical physical transport coefficients can be computed from the eigenvalues of the Liouville equation of the dynamical system it was found that, for a certain class of chaotic dynamical systems, transport coefficients are fractal functions of respective control parameters such as particle density, temperature, or field strength [Kla95, Kla96, Kla99a, Gas98c, Har01, Gro02, Kor02]. This phenomenon reflects on a macroscopic scale the topological instability of the chaotic equations of motion under parameter variation. Deterministic diffusion coefficients can alternatively be computed from periodic orbit theory yielding elegant formulas linking diffusion to the stability of the cycles of dynamical systems trajectories [Cvi95, Cvi92, Gas98a, Cvi03].

Much work has been devoted to understand the nonequilibrium entropy production in simple chaotic model systems such as two-dimensional *multibaker maps* and *periodic Lorentz gases*. Tél, Vollmer, Breymann and Matyas

¹The acronym holds for the initials of Sinai, Ruelle, and Bowen.

[Bre96,Tel96,Vol97,Bre98,Vol98,Tel00,Vol00,Mat01,Vol02,Vol03] as well as Gaspard, Tasaki, Dorfman and Gilbert [Gas97,Gil99a,Tas99,Tas00,Gil00a,Gil00b,Dor02] have proposed new concepts for defining coarse-grained Gibbs entropies leading to an entropy production of nonequilibrium processes which is in agreement with irreversible thermodynamics. The former group attributed the source of irreversible entropy production to the chaotic mixing of the dynamical system and to the associated loss of information due to the coarse graining. The latter authors argued that the singularity of the SRB measures exhibited by these nonequilibrium systems enforces a respective coarse graining for mathematical reasons. Hence, the source of irreversible entropy production is identified with the fractal character of these SRB measures. Cohen and Rondoni, on the other hand, criticized both approaches due to the fact that the simple models analyzed so far consist of moving point particles that do not interact with each other but only with some fixed scatterers [Coh98,Ron00a,Coh02,Ron02b]. In their view these systems are non-thermodynamic models that do not allow to identify local thermodynamic equilibrium or any proper source of thermodynamic entropy production; however, see the replies of the criticized authors in Refs. [Vol02,Dor02,Tel02,Gas02,Gas03].

To conclude this brief outline of the Hamiltonian dynamical systems approach to nonequilibrium steady states we refer to an interesting experiment that was proposed and carried out by Gaspard et al. [Gas98b,Bri01]. Its purpose was to verify the existence of microscopic deterministic chaos in the dynamics of a real interacting many-particle system. Long trajectories of a tracer particle suspended in a fluid were recorded, and this data was used for computing a coarse grained entropy that was argued to yield a lower bound for the sum of positive Lyapunov exponents of the system. However, after this work was published non-chaotic counterexamples were constructed yielding almost indistinguishable results for the coarse-grained entropy [Det99b,Gra99,Det00b]. This initiated ongoing discussions and motivated research on transport in non-chaotic models, which complements existing results for chaotic systems [Lep00,Cen00,Cec03,Alo02,Gra02].

B. The thermostated dynamical systems approach to nonequilibrium steady states

A nontrivial limitation of the Hamiltonian approach to chaotic transport is that it excludes nonequilibrium constraints generating a continuous flux of energy into the system as, for example, the application of external fields.² Such situations necessitate the modeling of an infinite dimensional *thermal reservoir* that is able to continuously absorb energy in order to prevent a subsystem from heating up [Pen79,Rue99b,Gal99,Dor99,Ron02a]. The need to model these situations emerged particularly from *nonequilibrium molecular dynamics computer simulations* that focus on simulating heat or shear flow of many-particle systems or currents under application of external fields [Eva90b,Hoo91,Hes96a,Mor98,Hoo99,Det00a,Mun00,Tuc00].

A well-known example for modeling thermal reservoirs is provided by the *Langevin equation* [Lan08] yielding the interaction with a heat bath by a combination of Stokes friction and stochastic forces [Wax54,Rei65,Pat88,Kub92,Zwa01]. Indeed, one way to derive generic types of Langevin equations starts from a Hamiltonian formulation for a heat bath consisting of infinitely many harmonic oscillators. This heat bath suitably interacts with a subsystem that consists of a single particle [Zwa73,For87,Kub92,Stu99,Zwa01]. In the course of the derivation the detailed bath dynamics is eliminated resulting in an equation of motion for the subsystem that is *stochastic and non-Hamiltonian*. The Langevin equation thus nicely illustrates Ruelle's statement “if we want to study non-equilibrium processes we have thus to consider an infinite system or non-Hamiltonian forces” [Rue99a].³

As we will argue in this review on various occasions, there is nothing mysterious in modeling thermal reservoirs with non-Hamiltonian equations of motion, see also, e.g., Refs. [Pen79,Sma80,Rue99b,Che95,Rue96,Che97] [Gal99,Lie99a,Ron02a]. In case of thermostated systems the non-Hamiltonianity results straightforwardly from projecting out spurious reservoir degrees of freedom, as we will outline in this review on several occasions. Early nonequilibrium molecular dynamics computer simulations actually employed stochastic models

²Note that the use of *Helfand moments* enables an indirect treatment of such situations similar to the use of equilibrium time correlation functions related to Green-Kubo formulas [Dor95, Gas98a].

³For a related statement see, e.g., Smale [Sma80]: “We would conclude that theoretical physics and statistical mechanics should not be tied to Hamiltonian equations so absolutely as in the past. On physical grounds, it is certainly reasonable to expect physical systems to have (perhaps very small) non-Hamiltonian perturbations due to friction and driving effects from outside energy absorbtion. Today also mathematical grounds suggest that it is reasonable to develop a more non-Hamiltonian approach to some aspects of physics.” In his interesting article Smale further suggests to “revive the ergodic hypothesis via introduction of a dissipative/forcing term” into Hamiltonian equations of motion, since in his view dissipative dynamical systems have a better chance to be ergodic than Hamiltonian ones that usually exhibit profoundly non-ergodic dynamics due to a mixed phase space.

of heat baths [And80,Cic80,Sch78,Ten82,All87,Nos91], however, very soon people started to look for alternatives. Infinite-dimensional Hamiltonian thermal reservoirs can very well be modeled and analyzed analytically [Eck99b,Eck99a,Zwa01], but on a computer the number of degrees of freedom must, for obvious reasons, remain finite. These constraints provided a very practical motivation for constructing nonequilibrium steady states on the basis of finite-dimensional, deterministic, non-Hamiltonian equations of motion.

About twenty years ago Hoover et al. [Hoo82] and Evans [Eva83a] independently and simultaneously came up with a strikingly simple non-Hamiltonian modeling of a thermal reservoir, which they coined the *Gaussian thermostat* [Eva83b]. This scheme introduces a (Gaussian) constraint in order to keep the temperature for a given subsystem strictly constant in nonequilibrium at any time step. A few years later Nosé invented a very related non-Hamiltonian thermal reservoir that was able to thermostat the velocity distribution of a given subsystem onto the canonical one in equilibrium, and to keep the energy of a subsystem constant on average in nonequilibrium [Nos84a,Nos84b]. His formulation was simplified by Hoover [Hoo85] leading to the famous Nosé-Hoover thermostat [Eva90b,Hoo91,Hes96a,Mor98,Hoo99,Det00a,Mun00,Ron02a]. Suitable adaptations of these schemes to nonequilibrium situations such as, e.g., shear flows yielded results that were well in agreement with predictions of irreversible thermodynamics and linear response theory [Eva90b,Sar98]. Hence, these thermostats became widely accepted tools for performing nonequilibrium molecular dynamics computer simulations. Eventually, they were successfully applied even to more complex fluids such as, for example, polymer melts, liquid crystals and ferrofluids [Hes96a,Hes96b,Hes97], to proteins in water and to chemical processes in the condensed matter phase [Tuc00].

Soon it was realized that this non-Hamiltonian modeling of thermal reservoirs not only enabled to efficiently construct nonequilibrium steady states on the computer but also that it made them amenable to an analysis by means of dynamical systems theory [Eva90b,Hoo91,Mar92a,Mar97,Tel98,Mor98,Hoo99]. First of all, in contrast to the stochastic Langevin equation Gaussian and Nosé-Hoover thermostats preserve the deterministic nature of the underlying Newtonian equations of motion. Even more, though the resulting dynamical systems are dissipative, surprisingly the thermostated equations of motion are still time-reversible hence yielding a class of systems characterized by the, at first view, contradictory properties of being *time-reversible, dissipative* and, under certain circumstances, even being *ergodic* [Che95,Che97,Hoo96b]. Computer simulations furthermore revealed that subsystems thermostated that way contract onto *fractal attractors* [Hol87,Mor87a,Mor87b,Hoo87,Pos88,Hoo88a,Mor89a,Pos89,Mor89b] with an *average rate of phase space contraction that is identical to the thermodynamic entropy production* [Hol87,Pos88,Che93a,Che93b]. This led researchers to conclude that in thermostated dynamical systems the phase space contraction onto fractal attractors is at the origin of the second law of thermodynamics [Hol87,Rue96,Rue97b,Rue97a,Hoo99,Rue99b,Gal98,Gal99,Rue03].

Interestingly, the average rate of phase space contraction plays the same role in linking statistical physical transport properties to dynamical systems quantities as the escape or decay rates in the Hamiltonian approach to nonequilibrium [Tel96,Rue96,Bre98,Gil01]. The key observation is that, on the one hand, the average phase space contraction rate is identical to the sum of Lyapunov exponents of a dynamical system, whereas, on the other hand, for Gaussian and Nosé-Hoover thermostats it equals the thermodynamic entropy production. For thermostated dynamical systems this again furnishes a relation between transport coefficients and dynamical systems quantities [Mor87a,Pos88,Eva90a,Van92,Bar93,Coh95,Eva00,Aok02]. A suitable reformulation of these equations makes them formally analogous to the ones obtained from the Hamiltonian approach to transport. These results were considered as an indication for the existence of a specific backbone of nonequilibrium transport in terms of dynamical systems theory [Tel96,Bre98,Gas98a,Gil01].

Another interesting feature of Gaussian and Nosé-Hoover thermostated dynamical systems is the existence of *generalized Hamiltonian and Lagrangian formalisms* from which the thermostated equations of motion can be deduced, which involve non-canonical transformations of the phase space variables [Nos84a,Nos84b,Det96b,Det97a,Mor98,Cho98]. Similarly to Hamiltonian dynamics deterministically thermostated systems often share a certain symmetry in the spectrum of their Lyapunov exponents known as the *conjugate pairing rule*, which was widely studied in the recent literature [Dre88,Pos88,Eva90a,Sar92,Gup94,Coh95,Det95,Del96b,Det96c,Lat97,Del97b,Del97a][Det97a,Mor98,Sea98,Bon98b,vB98,Woj98,Rue99b,vB00b,Dol00,Pan02c,Pan02b,Pan02a,Mor02,Tan02b]. That is, all Lyapunov exponents of a given dynamical system can be grouped into pairs such that each pair sums up to the same value, which in nonequilibrium is non-zero. In most cases Lyapunov exponents of thermostated systems can only be calculated numerically. However, for the periodic Lorentz gas and related systems there is an elegant analytical approach by means of kinetic theory developed by van Beijeren and Dorfman et al. [vB95,vB96,Lat97,vB97,vZ98,vB98,vB00b]. Furthermore, in recent computer simulations of interacting many-particle systems Posch et al. [Mil98a,Pos00a,Mil02,Hoo02c,For03] observed the existence of *Lyapunov modes* in thermal equilibrium indicating that the microscopic contributions to the Lyapunov instability of a many-particle fluid form specific modes of instability, quite in analogy to the well-known hydrodynamic modes governing macroscopic transport [Eck00,McN01,Tan02c,Tan02a,Mar03].

All these interesting properties inspired mathematicians to look at these systems from a more rigorous point of view.

A cornerstone is the proof by Chernov et al. of the existence of Ohm's law for the periodic Lorentz gas driven by an external electric field and connected to a Gaussian thermostat [Che95,Che97]. Another important development was the *chaotic hypothesis* by Gallavotti and Cohen [Gal95a,Gal95b,Gal98,Gal99], which was motivated by results from computer simulations on thermostated dynamical systems [Eva93a].⁴ This fundamental assumption generalizes Boltzmann's ergodic hypothesis in summarizing some general expectations on the chaotic nature of interacting many-particle systems which, if fulfilled, considerably facilitate calculations of nonequilibrium properties.

Further promising achievements in the field of thermostated dynamical systems are *fluctuation theorems* that establish simple symmetry relations between positive and negative fluctuations of the nonequilibrium entropy production. Again, such laws first came up in the framework of nonequilibrium molecular dynamics computer simulations for thermostated systems, see Evans, Cohen and Morriss [Eva93a]. Later on respective theorems were proven by Gallavotti and Cohen starting from the chaotic hypothesis [Gal95a,Gal95b].⁵ Related theorems for stochastic systems were derived in Refs. [Kur98,Leb99]. In Ref. [Mae99] it was argued that fluctuation theorems can more generally be understood as an intrinsic property of Gibbs measures⁶ defined in nonequilibrium situations. Meanwhile fluctuation theorems have been verified for many different systems in many different ways analytically [Dor99,Rue99b,Ron00b,Jar00,Eva02b,Jep03], by computer simulations [Bon98a,Lep00,Eva02b,Sch03], and in physical experiments [Cil98,Wan02]. It appears that fluctuation theorems belong to the rather few general results characterizing nonequilibrium steady states very far from equilibrium thus generalizing Green-Kubo formulas and Onsager reciprocity relations, which can be derived from them nearby equilibrium [Gal96b,Gal98,Gal99,Eva02b,Gal03].

C. Outline of this review

This review focuses on the non-Hamiltonian approach to nonequilibrium steady states employing deterministic and time-reversible thermostats. However, even this part of chaotic transport theory became so large already that we had to make a rather restrictive choice concerning subjects which we cover here. Details of the Hamiltonian theory of transport will be discussed whenever respective crosslinks can be established, which is primarily the case concerning relations between transport coefficients, dynamical systems quantities and nonequilibrium entropy production.

Our presentation attempts to be rather pedagogical. In Chapter II we motivate thermostats in a very intuitive way that is particularly directed to non-experts. This motivation is supplemented by a more detailed analysis of the Langevin equation from the point of view of modeling thermal reservoirs. We then sketch briefly how to compute velocity distribution functions for a subsystem interacting with a thermal reservoir that consists of arbitrarily many degrees of freedom. This basic problem of equilibrium statistical mechanics illustrates the importance of suitably projecting out reservoir degrees of freedom, and the results will be used in Chapter VII for systematically constructing thermal reservoirs modeling an arbitrary number of degrees of freedom, as well as in Chapter VIII.

In the final section of Chapter II we define the periodic Lorentz gas, a standard model in the field of chaos and transport. In the following chapters this simple model will be driven by an external electric field and thermalized by applying some generic types of thermostats that we introduce step by step. The corresponding nonequilibrium steady states will be numerically constructed and analyzed concerning their statistical and chaotic dynamical properties. Applying a variety of different thermal reservoirs to the same model enables us to inquire about possible universal chaos and transport properties of nonequilibrium steady states generated by different thermostats. The question to which extent such universal properties exist forms the main theme of our review.

This discussion is put forward in Chapter III by introducing the *Gaussian thermostat*, which is the most simple and prominent example for modeling a deterministic and time-reversible thermal reservoir. Note that this scheme constrains the energy directly in the interior of a subsystem and not at some boundaries, hence it is called a *bulk thermostat*. We summarize what we consider to be the crucial properties of this class of thermostats as far as connections between transport properties and dynamical systems quantities are concerned.

Chapter IV features a discussion of the *Nosé-Hoover thermostat*, from which the Gaussian one is obtained as a special case, and some generalizations of it. We motivate the Nosé-Hoover thermostat starting from the (generalized) *Liouville equation* for dissipative dynamical systems which we briefly derive. The Nosé-Hoover scheme is conceptually

⁴The chaotic hypothesis, in its original formulation [Gal95b], states: *A reversible many-particle system in a stationary state can be regarded as a transitive Anosov system for the purpose of computing the macroscopic properties of the system.*

⁵For similarities and differences between Evans-Cohen-Morriss and Gallavotti-Cohen fluctuation theorems see, e.g., Refs. [Coh99,Ron02a,Eva02b].

⁶See, e.g., Refs. [Bec93,Dor99] for introductions to Gibbs measures.

analogous to the Gaussian one thus yielding analogous formulas relating chaos to transport. However, despite this formal analogy the fractal structure of the attractor of the Nosé-Hoover thermostated Lorentz gas changes differently under parameter variation in comparison to the Gaussian thermostated model. This is reflected in different bifurcation diagrams, and correspondingly we obtain different field dependencies of the electrical conductivity for both models. In Chapter V we present a critical assessment of chaos and transport properties of nonequilibrium steady states generated by these two well-known and widely used thermostating schemes as presented up to this point. A key feature is that the models of thermal reservoirs discussed so far exhibit a built-in identity between phase space contraction and thermodynamic entropy production. We take this opportunity to elaborate on the striking formal analogy between three formulas relating transport coefficients to dynamical systems quantities. Two of them are resulting from the Hamiltonian approach to transport for closed and open systems, one is emerging from the thermostated systems approach.

This enables us to pose more clearly the central question of this review, namely, whether there are universal statistical and chaotic dynamical properties of nonequilibrium steady states which are independent from the specific type of thermostat used. Partly this issue has been discussed in the literature under the label of *equivalence of nonequilibrium ensembles* related to different thermostats [Eva85b,Eva90b,Lie92,San92,Eva93b,Che95,Gal96a,Che97,Gal97,Coh98] [Sar98,Rue99b,vZ99,Det00a,Eva02a,Bon02,Hoo03,Gal03]. Additionally, there is a line of work arguing for an equivalence of ensembles between thermostated and non-thermostated time-discrete maps as far as nonequilibrium entropy production is concerned [Bre96,Tel96,Mor96b,Vol97,Bre98,Vol98,Gil99a,Gil99b,Tel00,Vol00,Vol02,Vol03].

Our critical discussion of standard thermostating schemes motivates to look for alternative models of thermal reservoirs, which will be introduced in the remaining chapters. The main idea is to construct thermal reservoirs that do not by default exhibit an identity between phase space contraction and entropy production. In order to be comparable to Gaussian and Nosé-Hoover schemes these alternative models must as well be deterministic and time-reversible, and one has to show that they generate well-defined nonequilibrium steady states. Sharing these properties they would provide counterexamples to the claimed universality of the identity as concluded from the analysis of standard Gaussian and Nosé-Hoover thermostats. Consequently, in this case also the relations between transport coefficients and dynamical systems quantities as derived for Gaussian and Nosé-Hoover thermostats would become different.

A first class of such counterexamples is presented in Chapter VI by what we call *non-ideal Gaussian and Nosé-Hoover thermostats* [Rat00a]. It follows a detailed discussion of their chaos and transport properties, again for the example of the driven periodic Lorentz gas. Chapter VII starts by reviewing a well-known thermostat acting only at the boundaries of a subsystem instead of in the bulk, which is known under the name of *stochastic boundary conditions* [Leb78,Cic80,Ten82,Gol85,Che95,Che97,Hoo98c,Pos98]. In order to compare this thermal reservoir to Gaussian and Nosé-Hoover thermostats we make stochastic boundaries deterministic and time-reversible leading to *thermostating by deterministic scattering*, a scheme that contains stochastic boundaries as a special case [Kla00b,Rat00b,Wag99,Rat02,Wag00]. As before, we first apply this deterministic thermal reservoir to the driven periodic Lorentz gas. However, in the final section of this chapter we also review results for shear and heat flow in a many-particle hard-disk fluid thermostated by deterministic scattering [Wag99,Wag00].

We will show that thermostating by deterministic scattering defines a second class of systems exhibiting nonequilibrium steady states in which phase space contraction is not necessarily equal to thermodynamic entropy production. Consequently, as in case of non-ideal Gaussian and Nosé-Hoover thermostats, there are no unique relations between transport coefficients and dynamical systems quantities anymore. Furthermore, related to the fact that this scheme defines boundary thermostats the spectra of Lyapunov exponents of dynamical systems thermostated that way yield properties that are rather different from the ones obtained for systems thermostated in the bulk by using Gaussian or Nosé-Hoover thermostats. Further systems with nonequilibrium steady states in which phase space contraction is not equal to entropy production have been explored in Refs. [Gas97,Coh98,Eck99a,Dae99,Gas98a,Ben01,Ron02a].

We finish our discussion in Chapter VIII by pointing towards a surprising connection between Nosé-Hoover thermostats and *active Brownian particles* as introduced by Schweitzer and Ebeling et al. [Sch98,Ebe99,Til99,Erd00]. The latter models are thought to mimick, among others, the crawling of isolated biological cells on rough surfaces which can be measured experimentally [Fra90,Sto91,Sch93,Har94,Die03]. Active Brownian dynamics is modeled by Langevin equations with velocity-dependent friction coefficients that enable a Brownian particle to convert internal into kinetic energy and *vice versa*. By using heuristic arguments we show that limiting cases of such models reduce to conventional Nosé-Hoover dynamics. Establishing this link to deterministic thermostats sheds some light onto the origin of so-called crater-like velocity distribution functions as they were previously observed in computer simulations for active Brownian particles. We argue that they may emerge as superpositions of canonical and microcanonical velocity distributions, a phenomenon that is nicely exemplified by the Nosé-Hoover thermostat under parameter variations.

The main conclusion of our review, summarized in Chapter IX, is that *from a dynamical systems point of view* conventional Gaussian and Nosé-Hoover thermostats provide only a very specific access road to the modeling of nonequilibrium steady states. A fundamental problem of these thermal reservoirs is that they furnish a default identity between the rates of average phase space contraction and thermodynamic entropy production, which is at the heart of

linking nonequilibrium thermodynamics to dynamical systems theory in case of non-Hamiltonian equations of motion. Our analysis shows that alternative, different types of thermostats lead to different such relations. Correspondingly, the associated fractal attractors, the Lyapunov spectra and even the field-dependent electrical conductivities may exhibit very different properties. The last result concerning transport coefficients, on the other hand, is contrasted by our example of an interacting many-particle system under shear and heat flow thermostated at the boundaries. Here all transport properties are very well in agreement with predictions from irreversible thermodynamics and linear response theory. Still, almost all of the chaotic dynamical properties of this system are profoundly different compared to systems that were thermostated by Gaussian or Nosé-Hoover schemes.

Consequently, one may suspect that the variety of different transport properties obtained for the driven periodic Lorentz gas when thermalized with different thermostats rather reflects the simplicity and the low dimensionality of the model. In other words, for simple systems consisting of non-interacting particles modifications of the equations of motion, e.g., by applying different thermostats, may indeed profoundly change their macroscopic transport properties. This aspect is particularly significant when the dynamical systems are *topologically unstable* leading, for example, to fractal transport coefficients, which are at variance with common expectations from nonequilibrium thermodynamics. In contrast, for interacting many-particle systems at least the *thermodynamic* properties appear to be rather independent from the type of thermostat used pointing towards an equivalence of ensembles as discussed by other authors. However, we emphasize that we do *not* find such an equivalence as far as the detailed *chaotic dynamical* properties of many-particle systems are concerned.

We thus conclude that the quest for universal characteristics of nonequilibrium steady states in dissipative chaotic dynamical systems is not yet over. At the moment the only candidate for a universal property of *deterministically thermostated systems*, as far as chaos properties are concerned, appears to be the *fractal structure of attractors*, whereas any further chaos and, depending on the simplicity of the model, even transport property might reflect the choice of the thermostat. This poses a challenge to find more general relations between chaos and transport properties in thermostated dynamical system than discussed up to now. For such an endeavor one may want to start from some suitably coarse-grained nonequilibrium entropy that does not measure details of phase space contraction which appear to be spurious if compared to, say, the Clausius entropy for which nothing else counts than the heat flux into the thermal reservoir. Despite the obvious importance of entropy production we avoid detailed discussions concerning the origin of the second law of thermodynamics. We believe this goes considerably beyond the level of this review, apart from the fact that there already exists a lot of profound literature on this subject, see, e.g., Refs. [Ger99,Bri95,Lie99b] and much further work mentioned in the course of this review.

As far as the style of discussion in this review is concerned we primarily appeal to physical intuition. That is, we keep things as simple as possible and do not present more technical details than absolutely necessary. This is reflected by the fact that there are only very few formulas but a lot of text, and quite a number of figures. We presuppose some basic knowledge of (nonequilibrium) statistical mechanics [Rei65,Hua87] and of dynamical systems theory [Sch89,Eck85,Ott93,Bec93,All97]. Mathematical concepts such as SRB measures and Anosov systems are not employed explicitly, despite the fact that all issues discussed in our review are intimately related to them. These objects do play a crucial role for building up a rigorous mathematical theory of nonequilibrium steady states as outlined, e.g., in Refs. [Gas98a,Dor99,Gal99,Rue99b]. However, here we work on a level that is less rigorous consisting of straightforward physical examples and demonstrations plus some simple calculations and results from computer simulations. It is our hope that this approach still suffices to make the reader familiar with what we believe are some central problems in this field. Parts marked with a * contain some more detailed information that may be skipped at a first reading. Particularly Chapters I to IV should be understandable to a general readership. Chapter V may be considered more difficult, however, it forms an important core of this review. Chapter VI should again be more easy, whereas Chapters VII and VIII are intermediate.

Concerning books and reviews that are closely related to the topic covered by this work we may recommend Refs. [Eva90b,Hes96a,Mor98,Nic98,Hoo99,Det00a,Ron02a] for further reading. There exists also a number of conference proceedings and related collections of articles which the reader may wish to consult [Mar92a,Mar97,Tel98,Kar00,Sza00,Gar02,Kla03]. It is not our goal to come up with a complete list of references covering this rapidly growing research area. Instead, we restricted ourselves to citing articles that we feel are especially relevant to the problems highlighted in this review. Still, this resulted in quite a large number of references. We furthermore remark that this review does not intend to give a full *historical* account of recent developments in chaos theory and nonequilibrium statistical mechanics; for this purpose see, e.g., Refs. [Bru76,Gle88,Cvi03,Uff01,Vol02]. Only on certain occasions we go a little bit into the historical depth. We finally remark that Chapters VI and VII of this review summarize a recent series of papers by the author and coworkers [Kla00b,Rat00b,Wag99,Rat00a,Rat02,Wag00] originating from Ref. [Kla00b]. Sections VI.A and VIII.B, on the other hand, contain new results that have not been published before.

II. MOTIVATION: COUPLING A SYSTEM TO A THERMAL RESERVOIR

In this chapter we build the bridge from the introductory section to the main part of this review by introducing some basic concepts, models and notations. We first outline, in a very heuristic way and from a very physical point of view, what thermal reservoirs or so-called “thermostats” are and explain why they are indispensable for studying steady states under typical nonequilibrium conditions.

We then briefly remind the reader of the well-known Langevin equation that may also be thought of modeling the interaction of a subsystem (in this case a single Brownian particle) with a thermal reservoir (the surrounding fluid). In particular, we outline a short derivation of the Langevin equation from Hamiltonian equations of motion in which the thermal reservoir is modeled as a collection of non-interacting harmonic oscillators. This way we exemplify two extreme cases of modeling thermal reservoirs, namely either by purely Hamiltonian dynamics or, alternatively, in terms of some simple but dissipative, irreversible and stochastic equations of motion.

After this discussion of the detailed microscopic dynamics we elaborate on the general functional forms of the velocity distribution functions of subsystem plus thermal reservoir in thermal equilibrium. By means of very simple statistical physical arguments we sketch how to calculate velocity distributions for a subsystem of d_s degrees of freedom which interacts with a d_r -dimensional thermal reservoir in an ideal equilibrium situation. In case of $d_r \rightarrow \infty$ these velocity distributions converge to their canonical counterparts. This simple problem illustrates the importance of projecting out reservoir degrees of freedom. The obtained information will be used later on in order to construct thermal reservoirs, and for finding necessary conditions concerning the existence of bimodal velocity distributions.

To the end of this chapter we define the periodic Lorentz gas, a standard model in the field of chaos and transport, and give some indication of its physical interpretations. In the remaining chapters we will apply different types of thermal reservoirs to the periodic Lorentz gas under nonequilibrium situations. The resulting nonequilibrium steady states we will compare with each other concerning their statistical and chaotic dynamical properties.

A. Why thermostats?

A common problem of thermostating is how to cool down a bottle of beer on a hot summer day [Rei65]. One option is to simply put the bottle of beer in a swimming pool. Microscopically, there emerges a transfer of energy between the molecules in the bottle of beer composing a fluid at temperature T_B and the water molecules in the swimming pool at temperature $T_P < T_B$. Here we define temperature operationally on the basis of equipartitioning of energy onto all available degrees of freedom [Rei65,Hua87] connecting temperature with the average kinetic energy of a system. Under the assumption that the water molecules are properly interacting with each other, in the sense that such an equipartitioning can properly be established, on average the excess energy related to the temperature difference $T_B - T_P$ will flow across the surface of the beer bottle into the surrounding fluid. Under the very same assumption, it will furthermore equally distribute onto all the water molecules. However, since the number of water molecules is extremely large the increase of the average temperature of the pool, in terms of the average kinetic energy per particle, will be negligibly small.

What we have sketched here is just the well-known process of classical thermal equilibration between a sufficiently small subsystem and a surrounding thermal reservoir, where both systems are initially at two different temperatures. After equilibration both systems will be approximately at the same temperature, $T_B \simeq T_P$. However, so far we have only discussed the simple case of relaxation to thermal equilibrium when subsystem and reservoir together form a closed system.

As a second, slightly more complicated example, think of a nonequilibrium situation in an open system such as a light bulb connected to a battery. The applied voltage will generate a current, and as an Ohmic resistance the thread in the bulb will exhibit some Joule heating. In a naive microscopic picture this heating may be understood as follows: The applied electric field will on average accelerate the electrons in the resistance. Consequently, if there were no mechanism for reducing their average kinetic energy the gas of electrons simply heats up, and no stationary current exists. On the other hand, the single electrons will collide with the atoms constituting the resistance. During these collisions they will exchange energy with the atoms, possibly in terms of exciting lattice modes and eventually causing the whole resistance to heat up. However, across its surface the resistance allows an average flow of energy into the surrounding medium by collisions between the atoms of the thread and the atoms or molecules of the gas. In case of the light bulb this flow of energy just causes the gas around the thread to glow.

The dissipation of energy into a thermal reservoir thus properly counterbalances the pumping of energy into the system by the external electric field and enables the system to evolve into a *nonequilibrium steady state (NSS)*. With that we mean that the statistical physical parameters describing the system on macroscopic scales are constant in time, despite the fact that the system is no longer in thermal equilibrium [dG62]. In case of our example, the existence of a

NSS implies that under the nonequilibrium condition of applying an external electric field the electron gas eventually exhibits a stationary current and that the temperature is constant. We note in passing that the proper definition of a nonequilibrium temperature is a subtle problem in itself [Rug97,Mor99], but operationally, again, the principle of equipartitioning of energy might be used [Pos88,Eva90b,Mor98,Hoo99]. If the existence of a NSS is due to the action of a thermal reservoir we say the system is properly *thermostated*.

In other words, thermostats are mechanisms by which the internal energy of a many-particle system, and thus its temperature, can be tuned onto a specific value. Any thermostat may be thought of being associated with some thermal reservoir consisting of an infinite number of degrees of freedom thus being large enough to absorb any amount of energy pumped into the system. Thermostats can be applied in order to achieve equilibration to a global thermal equilibrium or for sustaining a NSS in a nonequilibrium situation where there is a flux of energy through the system, such as induced by external fields or by imposing temperature or velocity gradients. In a similar vein, other constraints instead of fixing the temperature may be imposed onto a system leading, e.g., to constant pressure or constant stress ensembles [All87,Eva90b,Nos91,Hes96a,Tuc00].

The first question we must focus on before we elaborate on NSS is therefore: How can we suitably amend Newton's equations of motion in order to model an energy dissipation into a thermal reservoir? The basic problems involved here will be exemplified by means of the well-known Langevin equation. At this level of discussion restrict ourselves to equilibrium situations where the construction of thermal reservoirs may appear to be a rather technical problem. However, our main objective is to eventually apply thermal reservoirs as defined in equilibrium to nonequilibrium situations yielding NSS. In later chapters we will inquire to which extent the detailed properties of NSS depend on the detailed modeling of different thermal reservoirs, and to which extent they might be universal.

B. Stochastic modeling of thermal reservoirs: the Langevin equation

The Langevin equation [Lan08] provides a simple theoretical framework for describing what is known as *Brownian motion*: A sufficiently small particle immersed in a fluid performs irregular motion resulting from the collisions between the atoms or molecules of the medium and the particle [Rei65,Wax54,vK92,Pat88,Gal99]. For coal dust particles on the surface of alcohol this phenomenon was observed by the Dutch physician J. Ingenhousz in 1785. However, it became known more widely only later on by the work of the Scottish botanist R. Brown in 1827, who reported similar irregular movements of pollen grains under a microscope. The name Brownian motion was coined by A. Einstein in his famous work from 1905 describing this irregular motion in terms of diffusion processes. A related approach was already proposed by the French mathematician L. Bachelier in 1900 in order to understand the dynamics of stock values. Einstein's work led J.B. Perrin to the experimental measurement of the Avogadro number in 1908 and also motivated P. Langevin's modeling of Brownian motion published in the same year.⁷ We first briefly summarize some fundamental features of Langevin's stochastic approach to Brownian motion. In the following chapters we will repeatedly come back to these characteristic properties by discussing to which extent they are reproduced in deterministic chaotic models of Brownian motion.

According to Langevin a Brownian particle is randomly driven by instantaneous collisions with the surrounding particles. On the other hand, energy is removed from the system by some bulk friction. In one dimension this dynamics is modeled by amending Newton's equations of motion to

$$\begin{aligned} \dot{r} &= v \\ \dot{v} &= -\alpha v + \mathcal{F}(t) \quad , \end{aligned} \tag{1}$$

where r and v denote the position and the velocity of the Brownian particle. For convenience, here and in the following we set constants like the mass m of the particle and the Boltzmann constant k equal to one. \mathcal{F} holds for white noise, that is, a δ -correlated stochastic force with zero mean modeling the random collisions with the fluid particles, whereas α is a Stokes friction coefficient. In a steady state the molecular stochastic forces and the friction balance each other leading to the fluctuation-dissipation theorem [Rei65,Wax54,Pat88,Zwa01]

$$\alpha = \frac{1}{2T} \int_{-\infty}^{\infty} dt \langle \mathcal{F}(0)\mathcal{F}(t) \rangle \quad , \tag{2}$$

⁷For this short historical note on Brownian motion we largely followed the nice presentation in Ref. [Met00]; for more details see, e.g., Refs. [Bru76,Sta89].

where $\langle \dots \rangle$ denotes an ensemble average over the noise acting on the moving particles. The expression $C_{\mathcal{F}}(t) := \langle \mathcal{F}(0)\mathcal{F}(t) \rangle$ is an example of a correlation function. α is in turn related to the diffusion coefficient D of the Brownian particle according to the Einstein relation

$$D = T/\alpha \quad , \quad (3)$$

where T is the temperature obtained from equipartitioning of energy, $T = \langle v^2 \rangle$. D is defined independently via the mean square displacement,

$$D := \lim_{t \rightarrow \infty} \frac{\langle [x(t) - x(0)]^2 \rangle}{2t} \quad . \quad (4)$$

Here the angular brackets denote an equilibrium ensemble average over moving particles. Alternatively, D can be obtained from the Green-Kubo formula for diffusion

$$D = \int_0^\infty dt \langle v(0)v(t) \rangle \quad , \quad (5)$$

which is an exact transformation of Eq. (4) [Zwa01].

The Green-Kubo formula Eq. (5) and the fluctuation-dissipation theorem Eq. (2) are formally analogous in relating a macroscopic quantity characterizing the fluid to an integral over some correlation function. $C_v(t) := \langle v(0)v(t) \rangle$ is called the velocity autocorrelation function of the moving particle. As can easily be shown by solving the Langevin equation Eq. (1) for C_v , the velocity autocorrelation function decays exponentially in time thus ensuring that, in terms of the Green-Kubo formula Eq. (5), the diffusion coefficient exists.

If one considers the Brownian particle as a subsystem and the surrounding particles as an infinite dimensional thermal reservoir, the Langevin equation precisely models the situation where a subsystem suitably interacts with a thermal reservoir. However, so far we have motivated this equation purely heuristically. It is therefore interesting to discuss a simple derivation of the above Langevin equation that actually starts from a fully Hamiltonian modeling of subsystem plus thermal reservoir in which the heat bath consists of an infinite number of harmonic oscillators [Zwa73,For87,Kub92,Stu99,Zwa01].⁸ It nicely demonstrates what kind of simplifying assumptions one has to make, starting from first principles, in order to arrive at the simple modeling of thermal reservoirs in terms of Eq. (1).

Let the Hamiltonian of the Brownian particle be

$$H_s = \frac{v^2}{2} \quad (6)$$

and let the heat bath of harmonic oscillators be

$$H_B = \sum_j \left(\frac{v_j^2}{2} + \frac{\omega_j^2}{2} \left(x_j - \frac{\gamma_j}{\omega_j^2} x \right)^2 \right) \quad , \quad (7)$$

where the oscillators exhibit a special coupling to the subsystem. Here ω_j is the frequency of the j th oscillator and γ_j the strength of the coupling between the Brownian particle and the j th oscillator. The Hamiltonian equations of motion for the combination of subsystem plus thermal reservoir then read

$$\begin{aligned} \dot{x} &= v \\ \dot{v} &= \sum_j \gamma_j \left(x_j - \frac{\gamma_j}{\omega_j^2} x \right) \end{aligned} \quad (8)$$

$$\begin{aligned} \dot{x}_j &= v_j \\ \dot{v}_j &= -\omega_j^2 x_j + \gamma_j x \end{aligned} \quad . \quad (9)$$

The formal solution of the inhomogeneous differential equation of second order Eq. (9) reads

⁸In Ref. [Stu99] this model was attributed to Ford and Kac [For87], however, it already appears at least in the paper by Zwanzig [Zwa73]; see also further references in Ref. [For87].

$$x_j(t) = x_j(0) \cos(\omega_j t) + v_j(0) \frac{\sin(\omega_j t)}{\omega_j} + \gamma_j \int_0^t ds x(s) \frac{\sin(\omega_j(t-s))}{\omega_j} . \quad (10)$$

Performing integration by parts for the latter integral and thereafter putting Eq. (10) into Eq. (8) yields the formal Langevin equation

$$\dot{v}(t) = - \int_0^t ds K(s)v(t-s) + F(t) . \quad (11)$$

By comparing this equation to the former stochastic Langevin equation Eq. (1) the first term on the right hand side is identified as some nonlinear, non-Markovian friction containing the memory function

$$K(t) = \sum_j \frac{\gamma_j^2}{\omega_j^2} \cos(\omega_j t) . \quad (12)$$

The second term on the right hand side of Eq. (11) must consequently yield the “noise”, which is given explicitly by

$$F(t) = \sum_j \gamma_j v_j(0) \frac{\sin(\omega_j t)}{\omega_j} + \sum_j \gamma_j \left(x_j(0) - \frac{\gamma_j}{\omega_j^2} x(0) \right) \cos(\omega_j t) . \quad (13)$$

Note that $F(t)$ is fully deterministic in depending on the initial conditions of all heat bath variables.

In order to recover Eq. (1) both expressions are now simplified as follows: If the spectrum of frequencies ω_j is thought to be continuous, the memory function Eq. (12) may be written as a Fourier integral. By assuming convenient functional forms for the density of states of ω_j and for the coupling coefficients γ_j the memory function can be replaced by a delta function, $K(t) \sim \delta(t)$. In this special case the Langevin equation Eq. (11) is Markovian and the ordinary Stokes friction of Eq. (1) is recovered.

As far as the “noise” is concerned, according to Eq. (13) $F(t)$ is a linear function of the initial positions and velocities of all bath oscillators that are furthermore independent degrees of freedom. Hence, there are no correlations between these variables. If all initial conditions are *sampled randomly* from a canonical distribution one can show that the fluctuation-dissipation theorem takes the form [Zwa01]

$$\langle F(t)F(t') \rangle = T K(t-t') . \quad (14)$$

Under the above assumption that the memory function is Markovian this equation boils down to Eq. (2), or in other words, the fluctuations induced by $F(t)$ turn out to be white noise. We see that, in this case, the noise is put in “by hand” into Eq. (11) by assuming a suitable distribution of initial conditions for the heat bath variables.

In summary, we have discussed the connection between two extreme versions of modeling the interaction of a subsystem consisting of a single particle with a thermal reservoir: One employs the fully Hamiltonian, i.e., deterministic, time-reversible and phase space preserving equations of motion Eqs. (6) and (7). To start this way may be considered convenient from a microscopic point of view. However, note that the statistical properties of the harmonic oscillator heat bath are pre-determined by the choice of initial conditions supplemented by the specific form of the memory kernel in Eq. (14). The latter yields the decay of the force correlations, hence the problem of introducing randomness is shifted towards choosing a proper initial distribution for the oscillator variables. A realistic heat bath, on the other hand, should generate a (canonical) equilibrium distribution of position and velocity variables in a self-contained way, that is, due to the action of the dynamical system defining the bath and irrespective of any specific initial conditions. That this is not the case for the harmonic oscillator heat bath one may consider as quite a deficiency of the model. Another more practical disadvantage becomes clear in nonequilibrium situations, where the sum over harmonic oscillators in Eq. (7) must be infinite in order to allow for the existence of a NSS. Though taking this limit does not pose any crucial difficulty for analytical investigations, the Hamiltonian scheme thus becomes very inconvenient for computer simulations.

The alternative type of modeling consists of the very intuitive linear and Markovian Langevin equation Eq. (1). However, according to its derivation from the harmonic oscillator heat bath strictly speaking these nice properties emerge only because of profound approximations. Even more, the dynamics eventually turns out to be non-Hamiltonian, that is, stochastic, irreversible and, as a consequence of Stoke’s friction, on average phase space contracting; see also Ref. [Hoo99] for related arguments.

Hence, both types of heat bath models do not really capture the whole essence of the problem. Correspondingly, there is plenty of room for generalizations of modeling thermal reservoirs, in two directions: On the one hand, starting from some Hamiltonian equations of motion or respective toy models of dynamical systems one may wish to put the

derivation of equations modeling the action of a heat bath onto a small subsystem onto more general, rigorous grounds. This approach was pursued, e.g., in a line of work by Beck et al. [Bec87,Bec95,Bec96]. Here the analysis starts from a time-discrete version of the Langevin equation Eq. (1) in which randomness is generated by a deterministic chaotic map thus trying to understand to which extent deterministic chaos modeling reservoir degrees of freedom can mimick stochastic noise. In a similar vein, Just and Kantz et al. considered chaotic dynamical systems with time scale separation where the fast degrees of freedom may be related to the action of a thermal reservoir [Jus01,Jus03,Kan03]. Note that similar to Beck's approach they modeled thermal reservoirs by dynamical systems that consist of only very few degrees of freedom exhibiting a chaotic dynamics. By using projection operator techniques for the phase space densities of the dynamical system variables they studied to which extent the fast degrees of freedom can be replaced by stochastic noise acting on the slow variables of respective subsystems, and how the resulting equations of motion for the subsystems look like. A related problem was investigated by Eckmann et al., who mathematically analyzed the nonequilibrium properties of a chain of anharmonic oscillators coupled to two heat baths at different temperatures modeled by Hamiltonian wave equations [Eck99b,Eck99a].

As far as we can tell it is extremely hard to derive rigorous results for the dynamical properties of thermal reservoirs and the associated subsystems, even in equilibrium situations, by starting from first principles. We are not aware that yet there is a general theory for this problem. A major difficulty appears to be that the precise characteristics of the thermal reservoirs depend to quite some extent on the detailed nonlinear and non-Markovian properties of the underlying equations of motion. Thus, typically one has to employ profound approximations in order to come up with some general statistical description, as was already indicated above. In nonequilibrium situations the problem of characterizing steady states with respect to their chaotic and dynamical properties becomes even more peculiar, which connects to our respective discussion in the introduction.

As an alternative to a rigorous bottom-up approach one may therefore construct a variety of simple and successively more sophisticated models of thermal reservoirs, with the purpose to learn about the detailed statistical and dynamical properties of the associated equilibrium and nonequilibrium steady states generated by these models. One may then inquire about general characteristics that are valid for all these models. We emphasize that this top-to-bottom approach, of course, bears other risks. In particular, one may too quickly conclude from the fascinating properties of a specific toy model concerning universal features. But this can be cured by trying to construct counterexamples. Of course, this bottom-up approach towards the physics of steady states is of a very heuristic nature. Still, in order to qualify as thermal reservoirs all models have to fulfill certain basic criteria. In the following we will require that, like ordinary equations of motion of moving particles, they are deterministic, time-reversible, and that they are able to generate a NSS under nonequilibrium conditions.

However, some details are still missing. So far we have focused on the equations of motion of subsystem plus thermal reservoir only. We did not explicitly discuss the detailed properties of the associated probability densities of subsystem and thermal reservoir and how they should look like, at least in equilibrium situations. This will be performed in the following section.

C. Equilibrium velocity distribution functions for subsystem and thermal reservoir

In this part we shall look at a subsystem that is coupled to a thermal reservoir from a purely statistical point of view. That is, we do not assume any detailed knowledge about the underlying equations of motion. We are interested only in the probability densities for the velocities of the subsystem and of the thermal reservoir, which we call velocity distribution functions, in the general case of thermal equilibrium. We do not discuss the probability densities for the associated position coordinates of the degrees of freedom, since the action of the thermal reservoir primarily concerns an exchange of energy related to the velocities. Our goal is to assess how different dimensionalities of subsystem and thermal reservoir, if the reservoir is first thought to be finite dimensional, affect the functional forms of the corresponding velocity distribution functions.

In order to illustrate the general case we start by discussing the most trivial example, where subsystem and thermal reservoir each consist of only one degree of freedom. Afterwards we switch to the general situation in which there is a subsystem with d_s degrees of freedom interacting with a thermal reservoir of d_r degrees of freedom, where typically $d_s < d_r$, and where the total number of degrees of freedom is $d = d_s + d_r$.⁹

Let us consider a large collection of points in the full phase space of the system, which in general may be restricted by some boundary conditions. The equilibrium velocity distribution function $\rho \equiv \rho(v_1, v_2)$ for $d = 2$ is then defined

⁹This problem has been posed as an exercise in the book of van Kampen on p.11 [vK92].

with respect to this ensemble of points, which move according to the same equations of motion. It is the number of points one can find in the phase space volume element $dv_1 dv_2$ centered around the velocity vector (v_1, v_2) at time t divided by the size of this volume element and by the total number of points N of the ensemble. By integrating over the whole accessible phase space the velocity distribution is properly normalized to one.

Let us now assume that we are in an equilibrium situation where equipartitioning of energy holds between all degrees of freedom and that the total energy of subsystem plus reservoir is conserved. For sake of simplicity we may assume that there is only kinetic energy as, e.g., in a gas of hard spheres. Hence, all points in velocity space should be uniformly distributed on a circle of radius $v := \sqrt{v_1^2 + v_2^2}$, where for convenience we set $v \equiv 1$, see Fig. 1 for an illustration. Subsystem plus reservoir thus obey the microcanonical distribution

$$\rho(v_1, v_2) \sim \delta(1 - v_1^2 - v_2^2) . \quad (15)$$

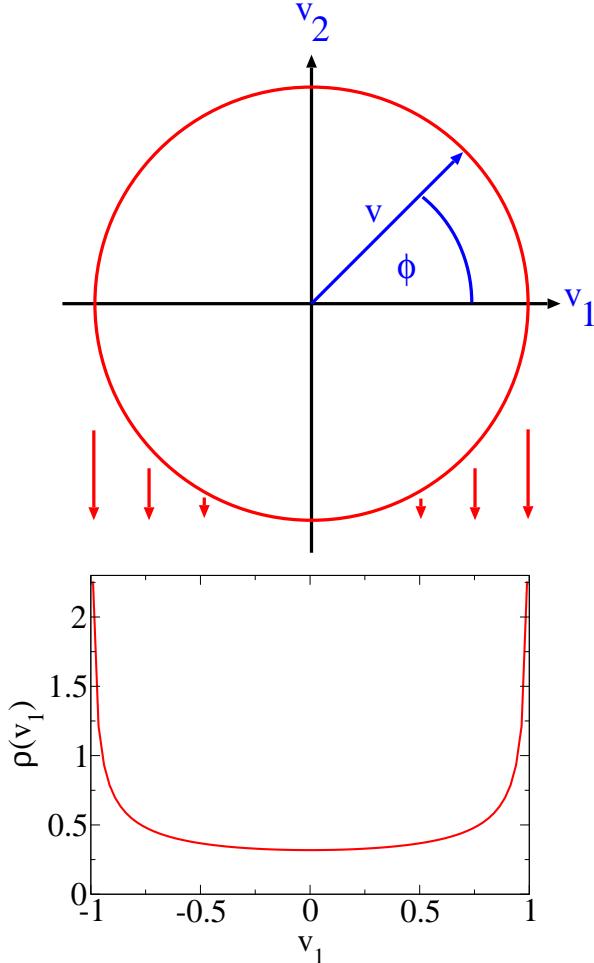


FIG. 1. Projection of the two-dimensional microcanonical velocity distribution Eq. (15) onto one component. The density of points is uniform on a circle of radius $v = 1$. The velocity vector is composed of the two velocity components v_1 and v_2 , and its direction is determined by the polar angle ϕ . The lower figure represents the one-component velocity distribution $\rho(v_1)$ Eq. (17) calculated from projecting out v_2 from Eq. (15).

It is now straightforward to calculate the velocity distribution functions of the subsystem, respectively of the thermal reservoir, which are obviously identical, by projecting out one of the two degrees of freedom from this microcanonical distribution. One way of how to do this is by using polar coordinates, $v_1 = \cos \phi$ and $v_2 = \sin \phi$, where ϕ denotes the polar angle in velocity space depicted in Fig. 1. The probability density corresponding to ϕ is then simply $\rho(\phi) = \text{const.}$ On the other hand, v_1 is a function of ϕ . According to conservation of probability the probability densities for v_1 and ϕ are related to each other by

$$\rho(\phi)|d\phi| = \rho(v_1)|dv_1| . \quad (16)$$

Hence, $\rho(v_1)$ is easily calculated in terms of $\rho(\phi)$ by differentiating v_1 leading to

$$\rho(v_1) = \frac{1}{\pi\sqrt{1-v_1^2}} , \quad (17)$$

where the prefactor is obtained from normalization. As indicated in Fig. 1, this result matches to physical intuition: By projecting the uniform distribution of points on the circle onto the v_1 -axis it is clear that there must be a higher density of points nearby the values of $v_2 = 0$ on the circle, whereas around $v_1 = 0$ the density of points must be minimal.

The main message of this trivial example is that non-uniform probability densities, which may otherwise be considered as an indicator of some non-Hamiltonian average phase space contraction, may very well coexist with a uniform, microcanonical one as it characterizes ordinary Hamiltonian dynamical systems. The obvious reason is that *one degree of freedom got projected out* respectively, so we neglected some information by not looking at the full combination of subsystem plus thermal reservoir.

Along the same lines and under the same conditions as described above, i.e., by assuming thermal equilibrium, equipartitioning of energy and a constant total kinetic energy E , the general case of a d_s -dimensional subsystem interacting with a d_r -dimensional thermal reservoir can now be studied. In this case the full velocity distribution function for subsystem plus thermal reservoir obeys the microcanonical distribution

$$\rho(v_1, \dots, v_d) \sim \delta(2E - v_1^2 - \dots - v_d^2) \quad (18)$$

with $d = d_s + d_r$ and v_k , $k = 1, \dots, d$, as all the velocities. That is, all points in velocity space are uniformly distributed on a hypersphere with radius $\sqrt{2E}$. How do the corresponding velocity distributions of subsystem and reservoir now look like for arbitrary numbers of degrees of freedom d , d_s and d_r ? Again, in order to calculate these distribution functions one has to project out the respective number of degrees of freedom from Eq. (18). Here we wish to focus on eliminating $d - 1$ or $d - 2$ degrees of freedom only. The solutions may be obtained along the same lines as in the two-dimensional case by using generalized spherical coordinates. However, we skip the calculations that are technically a bit more involved [Rat00b]. The results are as follows: By projecting out $d - 1$ dimensions the probability density for one velocity component v_1 is calculated to

$$\rho_d(v_1) = \frac{\Gamma(\frac{d}{2})}{\sqrt{\pi}\Gamma(\frac{d-1}{2})} \frac{(2E - v_1^2)^{\frac{d-3}{2}}}{(2E)^{\frac{d-2}{2}}} , \quad (19)$$

where $\Gamma(x)$ stands for the gamma function. This solution was already known to Maxwell and Boltzmann [Max79,Has09], however, in their calculation they took a different starting point; for an alternative derivation see also Ref. [Mil98b]. Projecting out $d - 2$ dimensions yields the probability density for the absolute value of the velocity vector of two components v_1 and v_2 with $v = \sqrt{v_1^2 + v_2^2}$ reading

$$\rho_d(v) = (d-2)v \frac{(2E - v^2)^{\frac{d-4}{2}}}{(2E)^{\frac{d-2}{2}}} . \quad (20)$$

These solutions are depicted in Fig. 2 for $d = 3, 4, 6$. As can be seen, for $d \gg 1$ both types of velocity distributions start to converge towards their canonical counterparts. This can be made precise by taking the limit of $d \rightarrow \infty$ in Eqs. (19) and (20). Using equipartitioning of energy, $E = \sum_{k=1}^d v_k^2 / 2 = Td/2$, where T is the temperature and $k_B \equiv 1$, we arrive at the well-known results

$$\lim_{d \rightarrow \infty} \rho_d(v_1) = \frac{1}{\sqrt{2\pi T}} e^{-v_1^2/2T} , \quad (21)$$

respectively

$$\lim_{d \rightarrow \infty} \rho_d(v) = \frac{1}{T} v e^{-\frac{v^2}{2T}} . \quad (22)$$

We have thus rederived the canonical distributions for v_1 and for v starting from the microcanonical one of subsystem plus thermal reservoir by projecting out an infinite number of reservoir degrees of freedom. Altogether the above equations yield the full information how, according to elementary equilibrium statistical mechanics, the velocity distribution functions of a subsystem consisting of d_s degrees of freedom shall look like if it experiences ideal interactions with a d_r -dimensional thermal reservoir.

We remark that the velocity distribution Eq. (21) is reproduced by an ensemble of particles obeying the stochastic Langevin equation Eq. (1) in the limit of $t \rightarrow \infty$. The corresponding Markov process modeling the stochastic behavior

of the velocity of a Brownian particle, which is characterized by a stationary Gaussian velocity distribution, is well-known in more mathematical terms as an Ornstein-Uhlenbeck process [vK92,Wax54].

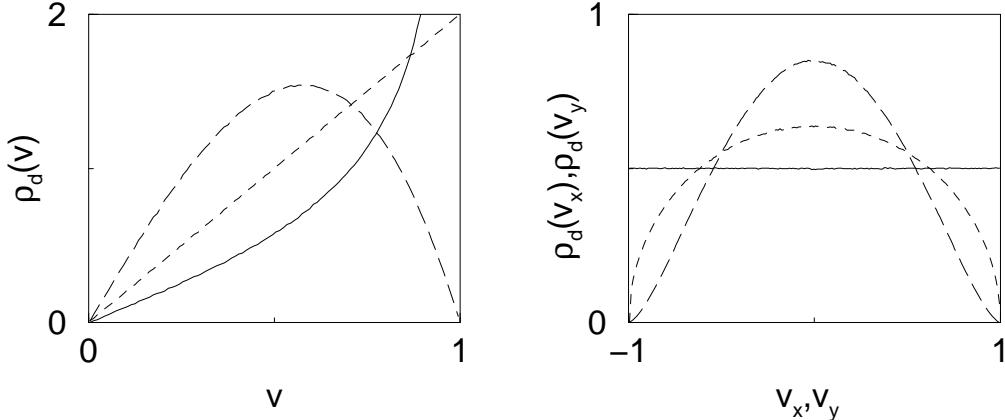


FIG. 2. Left: equilibrium velocity distribution function $\rho_d(v)$ for the absolute value v of the velocity vector (v_x, v_y) , which may be thought to represent a subsystem with two degrees of freedom coupled to a $(d-2)$ -dimensional thermal reservoir. Shown are $d = 3$ (solid curve), 4 (dashed curve) and 6 (long dashed curve) at a kinetic energy of $E = 0.5$ as calculated from Eq. (20). Right: analogous results for the single velocity components v_x , respectively v_y , calculated from Eq. (19).

An interesting question is now to which extent the above ideal functional forms of equilibrium velocity distributions are obtained for deterministic dynamical systems of d degrees of freedom when one looks at a respective smaller number of degrees of freedom $d_s < d$. A very popular example of this type of problem is the one- or two-dimensional harmonic oscillator coupled to a suitable deterministic thermal reservoir. If the reservoir mimicks an infinite number of degrees of freedom $d \rightarrow \infty$ the above derivations suggest that the harmonic oscillator velocities should simply approach canonical distributions. However, for such a behavior it is necessary that the thermostated subsystem exhibits at least an ergodic dynamics, because only in this case a single subsystem trajectory samples the whole phase space appropriately in order to possibly generate a canonical distribution. If the phase space is not uniquely accessible because of non-ergodicities the resulting velocity distributions will strongly depend on initial conditions and are typically not canonical. This discussion again indicates how sensitively the interplay between subsystem and thermal reservoir may depend on the detailed properties of the involved dynamical systems; for further details see Section IV.D.

As we already mentioned, the emphasis of this review is on nonequilibrium situations, and here thermal reservoirs are used as a tool to generate NSS representing transport properties of the associated dynamical system. Unfortunately, there is yet no analogue of microcanonical or canonical ensembles for nonequilibrium processes. In other words, nothing is known about how velocity distribution functions shall generally look like in nonequilibrium situations. The standard approach is therefore to define a thermal reservoir in an equilibrium situation by “gauging” it according to the requirement that it generates a microcanonical or a canonical velocity distribution for a respective subsystem connected to it. If this applies, a suitable nonequilibrium situation may be created.

For arbitrary deterministic dynamical subsystems it is by no means obvious or guaranteed that the thermal reservoir still properly “works” under these constraints, which intimately depends on the ergodic and chaotic dynamical properties of subsystem and thermal reservoir. If it does, the reservoir should generate a NSS that is characterized by specific nonequilibrium velocity distribution functions. This way, one can learn something about the variety of different velocity distributions that may exist in different nonequilibrium systems under application of specific models of thermal reservoirs, rather than the other way around. Unless there is a general theory of NSS starting from first principles, which at the moment is not the case, no other approach appears to be feasible here. Of course, for modeling nonequilibrium situations the associated thermal reservoirs must always mimick an infinite number of degrees of freedom in order to prevent a subsystem from heating up.

We finally remark that the above results for equilibrium velocity distributions of subsystems plus finite-dimensional thermal reservoirs will be used in Chapter VII in order to systematically construct a specific class of deterministic, time-reversible thermal reservoirs that dissipate energy according to inelastic collisions at the boundaries of a subsystem. Furthermore, we will use these results in Chapter VIII by discussing the origin of crater-like velocity distribution functions in models of active Brownian particles.

D. The periodic Lorentz gas

As we just discussed, whether or not thermal reservoirs are able to generate a specific velocity distribution for moving particles depends to quite some extent on the detailed dynamical properties of the subsystem to which it is applied. As an alternative to the problematic harmonic oscillator one may wish to choose a subsystem that is by default chaotic thus providing a more suitable starting point for the action of a thermal reservoir. Though chaotic one may wish that, nevertheless, this system is well analyzed in the mathematical literature.

Such a paradigmatic toy model is the *Lorentz gas*. The two-dimensional *periodic* version of it is sketched in Fig. 3 and consists of hard disks of radius R at density n whose centers are fixed on a triangular lattice in a plane. Between the scatterers a point particle moves with velocity \mathbf{v} and mass m by performing a free flight, whereas at collisions it exhibits specular reflections with the disks. If no further external constraints are applied the kinetic energy of the moving particle is constant, whereas the direction of the velocity changes according to the collisions with the scatterers. The phase space thus consists of the four variables (x, y, v_x, v_y) . However, because of energy conservation there are only three independent variables, where one may replace v_x and v_y by the angle of flight of the particle with the x -axis. For sake of simplicity we set $R = m = v \equiv 1$.

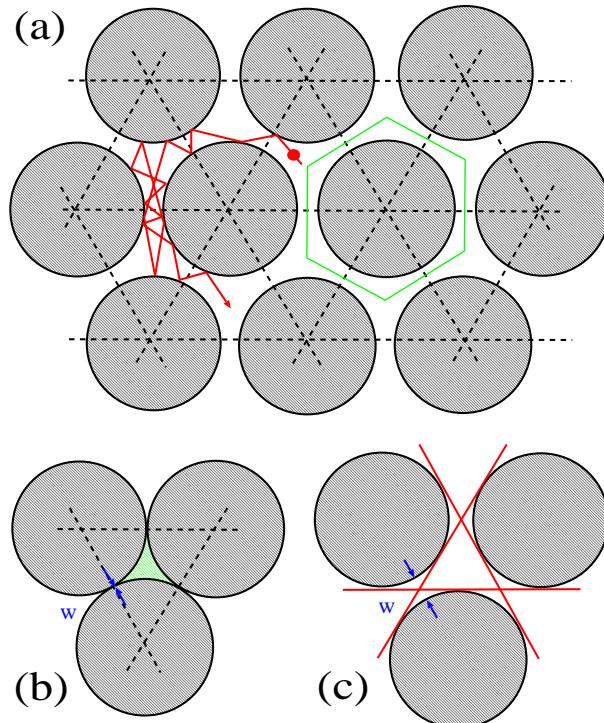


FIG. 3. Sketch of the two-dimensional periodic Lorentz gas where hard disks of unit radius are situated on a triangular lattice. (a) contains the hexagonal fundamental cell, or Wigner-Seitz cell, of this system. It also shows the trajectory of a point particle moving with a constant velocity and scattering elastically with the disks. (b) represents the limiting case of the highest density of scatterers where the minimal distance w between two scatterers is zero. That is, the scatterers touch each other and there is no diffusion. (c) depicts the other limiting case at a lower density where, for a specific value of w , for the first time trajectories exist along which a particle can move collision-free for an infinite time and thus sees an “infinite horizon”. In this case the dynamics is ballistic and the diffusion coefficient is infinite.

In the original work by H.A. Lorentz [Lor05], to whom the model is commonly attributed, the Lorentz gas consists of *randomly distributed hard spheres*. It was invented by him in 1905 in order to model the motion of classical electrons in metals, where the electrons do not interact with each other but scatter elastically only with hard spheres mimicking the atoms of the metal. However, as a laboratory device the two-dimensional periodic version of this system was, in a way, already introduced about 30 years earlier by Sir Francis Galton in 1877 [Gal77]. Hence, this model is also sometimes referred to as the *Galton board*. Galton used his device, which he called *the quincunx*, in lectures for demonstrating the existence of a binomial distribution that results when particles falling under the influence of a gravitational field are moving left or right through a periodic board of scatterers. He actually claimed that the same probabilistic laws existed in form of typical laws of heredity within populations of animate beings [Gal77]. His

theme is therefore very different from Lorentz' intention, who used his model to verify Drude's theory of classical electronic transport in metals [Dru00] by adding nonequilibrium constraints such as an electric field and a gradient of temperatures.

Though Drude's and Lorentz' work provide some heuristic microscopic derivation of Ohm's law, and of the law by Wiedemann and Frantz, it is well-known that this classical approach is not suitable to yield explanations for other fundamental properties of metals such as, e.g., their specific heat, which can only be understood by using quantum mechanics [Iba96]. On the other hand the two-dimensional Lorentz gas, the scatterers equipped with smooth potentials, turned out to be very useful for understanding electronic transport in *antidot lattices* under the action of electric and magnetic fields. These low-dimensional semiconductor devices can be manufactured with scatterers distributed both randomly and periodically in a plane. For small enough field strength the Fermi wavelength is smaller than the lattice constant. Hence, an electron exhibits an essentially classical transport process, where in good approximation the single electrons do not interact with each other; see Refs. [Wei91,Lor91,Wei97] for some experimental as well as Refs. [Gei90,Fle92] for corresponding theoretical work. We thus emphasize that much care has to be taken regarding the physical significance of the Lorentz gas concerning a general understanding of transport in real matter. The usefulness of this model for physically realistic situations should best be assessed from case to case. In this review we focus on the two-dimensional version of the Lorentz gas on a triangular lattice, so if not said otherwise with "Lorentz gas" we denote precisely this configuration of scatterers. The unit cell of this dynamical system, which is called *Wigner-Seitz cell* in solid state physics, is a hexagon, see Fig. 3 (a). Note that alternatively the scatterers may also be put on a square lattice, in which case the unit cell is sometimes called a *Sinai billiard* [Sin70]. If no further external constraints are added there is only one control parameter, which is the density of scatterers n or alternatively the smallest distance between two scatterers, the gap size w , as depicted in Fig. 3 (b) and (c). In the triangular case three different dynamical regimes are identified:

1. Particles are localized in space, i.e., they cannot leave a unit cell, since all disks touch each other, see Fig. 3 (b). This is the high density regime with a minimal gap size w between two adjacent disks of $w = 0$, and the diffusion coefficient is trivially zero.
2. There exist trajectories along which particles can move ballistically and collision-free for an infinite time, i.e., under certain initial conditions particles see "infinite horizons" in the Lorentz gas as indicated by Fig. 3 (c). This happens for $w > 4/\sqrt{3} - 2 \simeq 0.3094$ and marks the onset of a low-density regime in which the diffusion coefficient is infinite.
3. In-between these two regimes the horizon for the moving particles is finite. As has been proven in Refs. [Bun80,Bun81,Bun91,Che99], in this case a central limit theorem for the velocities exists and the diffusion coefficient is finite. This is related to an exponential decay of the velocity autocorrelation function of the moving particle [Mac83,Mat97] from which the existence of a diffusion coefficient follows according to the Green-Kubo formula for diffusion Eq. (5).

On this occasion we may refer to a further simple physical interpretation of the periodic Lorentz gas reflecting these three different dynamical regimes: The scattering of a point particle with a Lorentz gas disk may be looked at as a two-body problem, where a particle of a reduced mass μ moves with a relative velocity \mathbf{v} and scatters, in this case, with a hard core potential $V(R)$. By suitably rescaling the radii of the moving particle and of the fixed scatterer, whose sum should be constant, and by periodically continuing the unit cell including the moving particle, the dynamics may be considered as the collective motion of some lattice modes in a periodic medium such as a crystal. In this case the periodic Lorentz gas was coined the *correlated cell model* [Ald63,Del96a].

According to the three different regimes discussed above there are also three different regimes of lattice modes: In case 1 the lattice modes are again localized, in case 2 dislocations are possible, whereas case 3 may be interpreted as some kind of "melting". This relation of the periodic Lorentz gas to the correlated cell model was used to prove the existence of a shear and a bulk viscosity in what was called a "two-particle fluid" [Bun96]. Note also that, in kinetic theory, the random Lorentz gas is well-known as a model for a gas mixture of heavy and light particles, where the difference of the masses is large enough such that the heavy particles, in good approximation, can be considered to be immobile with respect to the light particles [Cha70].

The periodic Lorentz gas exhibits a number of important "nice" dynamical properties.¹⁰ First of all, it is Hamiltonian and thus deterministic, area-preserving and time-reversible. Secondly, it has been proven that the Lorentz gas is a K-

¹⁰For readers that are not too familiar with dynamical systems theory this paragraph may be skipped; alternatively, for respective definitions of dynamical systems quantities we refer to Refs. [Sch89,Ott93,Gas98a,Dor99].

system, which implies that it is mixing and ergodic [Bun80,Bun81,Bun91,Che99]. Furthermore, due to the defocusing character of the hard disks¹¹ the Lorentz gas is a hyperbolic, chaotic dynamical system. However, because of the hard walls it is not differentiable, as is exemplified by the existence of tangent collisions, and therefore strictly speaking it is not Anosov or Axiom A [Gas96, Gas98a]. Finally, corresponding to the three independent variables of the periodic Lorentz gas there are three different Lyapunov exponents reflecting its hyperbolic behavior: One is zero, which is the one parallel to the flow, the other two are smaller respectively larger than zero, and because the system is phase space preserving all Lyapunov exponents trivially sum up to zero.

We remark that for random configurations of scatterers in two and three dimensions the Lyapunov exponents have been computed analytically by means of kinetic theory, partly in comparison with results from computer simulations [vB95,Lat97,vB97,Del97b,vB98]. For the two-dimensional periodic Lorentz gas both on a quadratic and on a triangular lattice computer simulation results for the Lyapunov exponents were presented in Refs. [Gas95a, Gas98a]. Random and periodic Lorentz gases are prototypical models of so-called *particle billiards* that have been widely studied in the field of chaos and transport both from the physical as well as from the mathematical side of dynamical systems theory. Hence there exists a large literature that the reader may wish to consult in order to learn about more detailed properties, see, e.g., Refs. [Gas98a,Dor99,Sza00] and further references therein.

E. Summary

1. We started this chapter by elaborating on the physical meaning of a thermal reservoir. This discussion was performed on a very elementary heuristic level. The action of a thermal reservoir on a subsystem was first outlined for thermal equilibrium. In nonequilibrium situations thermal reservoirs are generally indispensable in order to generate NSS.
2. As a well-known example for modeling thermal reservoirs we have heuristically introduced the simplest form of a stochastic Langevin equation. We have also briefly summarized some of its most important properties. It was then shown how this Langevin equation can be derived starting from Hamiltonian equations of motion, where the heat bath is modeled by a collection of non-interacting harmonic oscillators. On this basis we have discussed deficiencies of both schemes as far as the modeling of thermal reservoirs is concerned, and we have mentioned some more recent approaches that try to go beyond this simple modeling.
3. On a more statistical level, we have outlined how to calculate the equilibrium velocity distribution functions for a single velocity component as well as for the absolute value of two velocity components for a subsystem that is coupled to a d_r -dimensional thermal reservoir. In the limit of $d_r \rightarrow \infty$ we recovered the corresponding well-known canonical distributions, as was to be expected. We indicated that these “ideal” velocity distribution functions, according to equilibrium statistical mechanics, may not by default be properly reproduced by an arbitrary deterministic dynamical subsystem such as the harmonic oscillator, coupled to some model of a thermal reservoir. Related problems for modeling NSS were also briefly discussed.
4. Finally, we introduced a simple deterministic dynamical system, the periodic Lorentz gas, which exhibits “nice” dynamical properties in an equilibrium situation by being, among others, Hamiltonian, mixing and fully chaotic. We started with a brief history of the (periodic) Lorentz gas, discussed its physical significance and some possible physical interpretations as far as physical reality is concerned. We classified its three different dynamical regimes and very briefly summarized its most important mathematical properties. In the following, the periodic Lorentz gas will serve as our standard model in order to compare the action of different thermal reservoirs with each other, particularly in nonequilibrium situations.

III. THE GAUSSIAN THERMOSTAT

We now introduce a very popular deterministic and time-reversible modeling of a thermal reservoir which is known as the *Gaussian thermostat*. We assign this thermostating scheme to the periodic Lorentz gas driven by an external electric field and summarize what we consider to be the most important features of the resulting model from a dynamical systems point of view. The properties we report are to a large extent typical for Gaussian thermostated

¹¹This type of scatterers is said to be *convex*, or *dispersing*.

systems altogether. Specifically, we review a connection between thermodynamic entropy production and the average phase space contraction rate as well as a simple functional relationship between Lyapunov exponents and transport coefficients. Furthermore, there exists a fractal attractor in the Gaussian thermostated Lorentz gas which changes its topology under variation of the electric field strength. Correspondingly, the electrical conductivity is an irregular function of the field strength as a control parameter. We also briefly elaborate on the existence of linear response in this model.

A. Construction of the Gaussian thermostat

In the following chapters the periodic Lorentz gas serves as a standard model to which different thermal reservoirs are applied. A big advantage of the Lorentz gas, say, in comparison to the harmonic oscillator is that it exhibits deterministic chaos, which is a consequence of the defocusing geometry of the scatterers. Hence, in contrast to the Langevin dynamics of Eq. (1) we do not need to impose a stochastic force onto this model in order to enforce Brownian motion-like spatial fluctuations for a moving particle.¹² Instead, some random-looking trajectories in position space are generated due to the intrinsic Lyapunov instability of the system, see again Fig. 3. This is in turn intimately related to the mixing and ergodic properties of the Lorentz gas. We thus replace stochasticity by deterministic chaos in order to generate a Brownian motion-like dynamics, cp. also to our discussion in Section II.B.

As was outlined in the previous chapter, in a certain regime of densities of scatterers the periodic Lorentz gas exhibits normal diffusion related to an exponential decay of the velocity autocorrelation function, in analogy to the diffusive properties of Langevin dynamics. In this review we do not study how the Lorentz gas dynamics changes under variation of the density of scatterers, see Refs. [Kla00a,Kla02c]. Instead, we simply choose one specific parameter value for the minimal distance between two scatterers, $w \simeq 0.2361$, as it is standard in the literature to ensure that a diffusion coefficient exists [Mor87a,Llo94,Llo95,Del95a,Mor96a,Det96a].

In order to drive this model out of equilibrium we apply an external electric field that, if not said otherwise, is parallel to the x -axis. However, as explained before, if there were no interaction with a thermal reservoir any moving particle would on average be accelerated by the external field consequently leading to an ongoing increase of energy in the system, and there were no NSS. Therefore the model must be connected to some thermal reservoir. In other words, it must be thermostated. The periodic Lorentz gas amended by an external field and coupled to a suitable thermal reservoir is called the *driven periodic Lorentz gas*. This model has been widely studied in the literature over the past fifteen years [Mor87a,Hoo88a,Hoo89b,Hoo92,Van92,Che93a,Che93b,Bar93,Lue93,Llo94,Llo95,Det95,Del95a] [Mor96a,Det96a,Det97b,Det97c,Bon97,Coh98,Mor98,Hoo98c,Hoo99,Dor99,Tel00,Bon00,Det00a,MM01,Bon02,Vol02] [Lar03].

Following our discussion of the Langevin equation one may remove energy from the field-driven Lorentz gas according to

$$\begin{aligned}\dot{\mathbf{r}} &= \mathbf{v} \\ \dot{\mathbf{v}} &= \boldsymbol{\varepsilon} - \alpha(\mathbf{v})\mathbf{v} \quad ,\end{aligned}\tag{23}$$

supplemented by the geometric boundary conditions imposed by the Lorentz gas scatterers. With $\alpha \equiv \alpha(\mathbf{v}) = \text{const.}$ we have an ordinary Stokes friction term, and the equations represent a deterministic variant of the stochastic Langevin equation Eq. (1) amended by an external electric field $\boldsymbol{\varepsilon}$. Here and in the following the electric charge q of the particle is set equal to one. This viscous Lorentz gas has been studied by computer simulations in Ref. [Hoo92].

For numerical solutions one has to discretize Eqs. (23) in time. The second of the above two equations then reads

$$\mathbf{v}(t + \Delta t) = \boldsymbol{\varepsilon}\Delta t + \tilde{\alpha}\mathbf{v}(t) \quad , \quad 0 < \Delta t \ll 1 \quad ,\tag{24}$$

with $\tilde{\alpha} := 1 - \alpha\Delta t$. For small enough Δt there is $0 < \tilde{\alpha} < 1$, and by keeping the time interval fixed the viscous force amounts to a rescaling of the velocity periodically in time with a constant scaling factor $\tilde{\alpha}$. This procedure can be made more efficient by replacing $\tilde{\alpha}$ according to

$$\tilde{\alpha}(\mathbf{v}) := \sqrt{\frac{E}{E(t)}} \quad ,\tag{25}$$

¹²On the other hand, without applying an external field the absolute value of the velocity for the moving particle is yet constant in the Lorentz gas, which is at variance to ordinary Langevin dynamics. However, see Chapter IV for respective further modifications of the Lorentz gas.

where E is the target kinetic energy of the system and $E(t)$ the measured kinetic energy at time t . The scaling factor now depends on the velocity of the moving particle and may thus fluctuate in time. This elementary but rather convenient numerical method to keep the energy fixed became well-known for molecular dynamics computer simulations under the name of *velocity rescaling* [Eva83a,All87,Hol87,Hol95,Hes96a,Hes96b,Hoo97,Det00a]. Note that both the Lorentz gas with a Stokes friction coefficient and with rescaled velocities is deterministic but not time-reversible.

In order to further improve the efficiency of these thermostating mechanisms one may start directly from a velocity-dependent friction coefficient in Eq. (23), $\alpha \equiv \alpha(\mathbf{v})$. Requiring energy conservation at any time step implies $d\mathbf{v}^2/dt = 0$ as a constraint on the functional form of $\alpha(\mathbf{v})$ and yields

$$\alpha(\mathbf{v}) = \boldsymbol{\varepsilon} \cdot \mathbf{v}/v^2 . \quad (26)$$

This method of thermostating was proposed simultaneously and independently by Hoover and coworkers [Hoo82] and by Evans [Eva83a] in 1982. Performed in the limit of $\Delta t \rightarrow 0$, the velocity rescaling Eqs. (24), (25) is identical to the combination Eqs. (23), (26) [Eva83a,Hol87,Hol95,Hes96a,Hoo97,Det00a].

In contrast to ordinary Stokes friction that only reduces the kinetic energy, the velocity-dependent version Eq. (26) pumps energy into the system whenever the particle is moving opposite to the field. This friction is maximal when the velocity is parallel to the field, and it is zero when velocity and electric field are perpendicular to each other. Trivially, it is zero when the electric field is zero due to the fact that in the equilibrium periodic Lorentz gas a particle is moving with a constant absolute value of the velocity anyway. Still, in comparison to the friction of the deterministic, generalized Langevin equation Eq. (11) that was obtained starting from the heat bath of harmonic oscillators, such a generalization of ordinary Stokes friction may not be considered physically unreasonable.

Alternatively, Eq. (26) can be derived from Gauss' principle of least constraints [Eva83b,Eva90b,Mor98,Ron02a], which is a fundamental principle of classical mechanics.¹³ For this reason a velocity-dependent friction force that keeps the energy of a particle constant at any time step was coined the *Gaussian thermostat* [Eva83b]. Correspondingly, the Gaussian thermostat applied to the driven periodic Lorentz gas generates a microcanonical-like distribution in velocity space [Mor98].¹⁴

In fact, here we are constraining only the kinetic energy of the moving particle, therefore this version is sometimes further classified as the *Gaussian isokinetic thermostat*. For soft particles one may fix alternatively the total internal energy consisting of the sum of kinetic plus potential energy yielding the *Gaussian isoenergetic thermostat*, see Refs. [Eva90b,Mor98,Det00a,Ron02a] for these denotations. Suitably amended versions of the Gaussian thermostat can also be applied, for example, to many-particle systems under shear, see Chapter VII for further discussions.

Similar to the case of Stoke's friction which models the loss of energy of a moving particle into a surrounding viscous fluid one may associate with the Gaussian friction variable Eq. (26) some imaginary thermal reservoir that acts at any instant of time. Thus the Gaussian thermostat is another example of a so-called *bulk thermostat*. We remark that this physical picture contradicts the specific interpretation of the driven periodic Lorentz gas as a model for noninteracting electrons moving in a periodic crystal. Here one may expect that energy is only dissipated at the collisions with a scatterer and not during a free flight. However, the action of the Gaussian thermostat is conceptually fine if the Lorentz gas is considered as a two-particle fluid that is immersed into another fluid serving as a thermal reservoir. Let us furthermore remark that in Chapter VII we will introduce boundary thermostats for the Lorentz gas, where a particle exchanges energy with a thermal reservoir only at the collisions with a scatterer. On this occasion we will discuss similarities and differences to what we find for the Gaussian thermostated case summarized below.

Surprisingly, the equations of motion Eqs. (23) supplemented by Eq. (26) are time-reversible consequently modeling the, at first view, seemingly contradictory situation of a deterministic, time-reversible, dissipative dynamical system [Hoo96b]. As will be outlined in the following, under certain conditions the Gaussian thermostated driven Lorentz gas furthermore exhibits an ergodic and chaotic particle dynamics and corresponding well-defined NSS. In contrast to standard Stoke's friction and to stochastic thermostats the Gaussian scheme thus enables to elaborate on the fundamental problem how time-reversible, deterministic, microscopic equations of motion may generate macroscopic irreversible transport in nonequilibrium situations associated with energy dissipation.

¹³In contrast to d'Alembert's principle, for the Gaussian version the virtual displacements are acceleration terms instead of the positions of a moving particle.

¹⁴Note that in nonequilibrium the distribution of points on the energy shell is not uniform anymore reflecting the existence of an average current.

B. Fundamental relations between chaos and transport for Gaussian thermostated dynamical systems

We now analyse the Gaussian thermostated driven periodic Lorentz gas from a dynamical systems point of view and summarize what we consider to be the characteristic chaos and transport properties of this class of dynamical systems.

1. Phase space contraction and entropy production

A first fundamental property of Gaussian thermostated systems is obtained from computing their *average phase space contraction rate* defined by

$$\kappa := \langle \nabla \cdot \mathbf{F}(\mathbf{r}, \mathbf{v}) \rangle , \quad (27)$$

where $\mathbf{F}(\mathbf{r}, \mathbf{v})$ stands for the equations of motion of the system Eqs. (23) and the brackets denote an ensemble average. A straightforward calculation, by taking into account that α is a function of \mathbf{v} , yields

$$\kappa = - \langle \alpha \rangle \quad (28)$$

with α defined by Eq. (26), where $\kappa < 0$. Let us now rewrite this equation by introducing a nonequilibrium temperature T . If we want to do so by using equipartitioning of energy [Eva90b,Mor98,Hoo99] we need to know about the number of degrees of freedom of the system. The velocity space is two-dimensional, but one may argue that the energy constraint eliminates one degree of freedom of the system. However, this argument is debatable, and actually there is quite an ambiguity in defining a temperature for the driven Lorentz gas [Che93a,Che93b].¹⁵ By assuming that there is one degree of freedom only we arrive at

$$v^2 = T , \quad (29)$$

with $k_B \equiv 1$. We can now write

$$-\kappa = \varepsilon \cdot \langle \mathbf{v} \rangle / T , \quad (30)$$

where the right hand side is the familiar expression related to the Joule heating derived from irreversible thermodynamics. Alternatively, one could have started from Clausius' definition of entropy production in terms of the heat transfer dQ between subsystem and thermal reservoir, $\Delta S = \int dQ/T$ [dG62,Hua87,Det00a,Gal03], yielding the same equation.¹⁶ We thus arrive at the fundamental result that, for Gaussian thermostated systems, there is an *identity between the absolute value of the average rate of phase space contraction and thermodynamic entropy production* [Hol87,Pos87,Pos88,Eva90b,Che95,Che97,Che93a,Che93b,Vol97,Bre98,Gil99a,Hoo99,Det00a,Vol03]. A third way to obtain this identity starts from Gibbs' definition of entropy production, as will be discussed in Chapter V.

2. Lyapunov exponents and transport coefficients

Note that Eq. (30) provides a crucial link between dynamical systems properties, in terms of phase space contraction, and thermodynamics, in terms of entropy production. By employing this link a second fundamental property for Gaussian thermostated systems is easily derived as follows: First of all, there is an identity between the average phase space contraction of a dynamical system and the sum of Lyapunov exponents [Eck85,Gas98a]. For the driven Lorentz gas under consideration two Lyapunov exponents are zero, due to the energy constraint and assessing the neutral direction parallel to the trajectory of a moving particle. From the remaining two exponents one is positive and one is negative, at least for small enough field strength, see, for example the numerical results of Refs. [Llo95,Del95b,Det95,Det96a,Mor96a,Mor98]. Consequently we have

¹⁵If we switch back to the Lorentz gas without an external field we also, trivially, have energy conservation. However, here nobody would claim that the number of degrees of freedom is reduced respectively.

¹⁶In the d -dimensional case and for N particles there is a prefactor of $Nd - 1$ on the right hand side of Eq. (28), but this factor cancels with a respective prefactor on the right hand side of Eq. (29) such that the identity is preserved [Coh98]. Note also that the Clausius form is only valid for quasistatic processes in, at least, local thermodynamic equilibrium.

$$\kappa = \lambda_+ + \lambda_- . \quad (31)$$

Let us now replace the average current by introducing the field-dependent electrical conductivity $\sigma(\varepsilon)$ according to¹⁷

$$\langle \mathbf{v} \rangle =: \sigma(\varepsilon) \varepsilon , \quad (32)$$

where ε stands for the absolute value of the field strength. For sake of simplicity here we consider only the case of the field being parallel to the x -axis. Because of the symmetry of the two-dimensional model $\sigma(\varepsilon)$ is then a scalar quantity, whereas for general direction of the field strength one has to employ a tensorial formulation [Llo95]. Replacing the average current $\langle \mathbf{v} \rangle$ on the right hand side of Eq. (30) by Eq. (32) and the average phase space contraction rate κ on the other side by Eq. (31) we arrive at a simple relation between the conductivity $\sigma(\varepsilon)$ and the sum of Lyapunov exponents of the dynamical system,

$$\sigma(\varepsilon) = -\frac{T}{\varepsilon^2} (\lambda_+(\varepsilon) + \lambda_-(\varepsilon)) . \quad (33)$$

This important connection between transport coefficients and dynamical systems quantities was first reported by Posch and Hoover for a many-particle system with an external field [Pos88] and was called the *Lyapunov sum rule* later on [Eva90a]. For the driven periodic Lorentz gas its existence was rigorously proven in Refs. [Che93a,Che93b]. Eq. (33) can also be related to periodic orbits [Van92] and was studied in much detail numerically [Bar93,Llo95,Del95b]. Functional forms that are completely analogous to Eq. (33) also hold for many-particle systems and for other transport coefficients such as viscosity [Eva90a,Eva90b,Coh95,Sar98] and thermal conductivity [Aok02] under the necessary condition that heat is dissipated by Gaussian and related thermostats [Mor98].

The Lyapunov sum rule moved particularly into the center of interest starting from the work by Evans, Cohen and Morriss [Eva90a] who introduced a further simplification of it for systems with many degrees of freedom. The observation was that for dissipative many-particle systems the spectrum of Lyapunov exponents may exhibit a remarkable symmetry property [Pos88,Mor89a,Eva90a]. This was first reported for the case of a uniform viscous damping by Dressler [Dre88] and was later on called the *conjugate pairing rule*: If all non-zero Lyapunov exponents are ordered according to their values they can be grouped into pairs such that each pair sums up to precisely the same value. This pairing rule is well-known for Hamiltonian dynamical systems, however, here the Lyapunov exponents appear in pairs that always sum up to zero. Indeed, in phase space preserving dynamical systems it can be shown that conjugate pairing is a direct consequence of the symplecticity of the Hamiltonian [Eck85,Mei92,Abr94,Gas98a].

If conjugate pairing holds for the very different class of dissipative, thermostated systems it enables to replace the sum over the full spectrum of Lyapunov exponents which appears on the right hand side of Eq. (33) by the sum over one pair of exponents only. For higher-dimensional dynamical systems this drastically simplifies the computation of transport coefficients according to Eq. (33), since the total number of different exponents is here extremely large and the full spectrum is very hard to extract numerically. Instead, for a conjugate pair one may just choose the largest and the smallest Lyapunov exponent, where the largest exponent is typically not too difficult to get [Ben80,Wol85,Ott93]. The smallest one, in turn, is best computed by reversing the direction of time [Hoo88b,Eva90a,Coh95,vB96,Lat97,Sar98,Sea98,Tan02b].

However, note that the reversed trajectories still have to be constrained to the invariant set associated with the forward dynamics. As we will further explain in the following section, in dissipative systems this set is usually a *fractal attractor* that becomes a *fractal repeller* under time reversal, and it requires some additional numerical efforts to keep the trajectories in this now unstable region. From a computational point of view the Lyapunov sum rule Eq. (33) supplemented by conjugate pairing thus does not appear to provide a more efficient mean for computing transport coefficients than other existing standard procedures. For example, along the lines of Eq. (33) it were easier to compute the average value of the thermostating variable instead of any Lyapunov exponent, see Eqs. (28) and (31). Conjugate pairing was analytically proven to hold under certain conditions that particularly concern the specific form of the interparticle potential and the special type of deterministic thermostat used [Det96c,Det97a,Mor98,Woj98,Rue99b,Pan02a]; see also the kinetic theory calculations for the three-dimensional Gaussian isokinetic thermostated driven random Lorentz gas in Refs. [Lat97,vB98,vB00b] and the respective comparison to computer simulations [Del97b]. Conjugate pairing in the three-dimensional driven periodic Lorentz gas, again connected to a Gaussian isokinetic thermostat, was numerically corroborated in Refs. [Det95,Mor96a].

¹⁷Strictly speaking this quantity may rather be called the *mobility* of a particle, in distinction from the conductivity that involves the charge and the density per unit volume of the mobile electrons of a conductor [Wan66,Rei65]. However, in our case there is no difference.

For interacting many-particle systems under shear the situation concerning the validity of conjugate pairing appears to be considerably less clear, see Refs. [Eva90a,Coh95,Gup94,Mor98] and the very recent discussion in Refs. [Mor02,Tan02b,Pan02b,Pan02c]; see also Refs. [Del96b,Sar92,Sea98] for numerical studies of various thermostated systems in which conjugate pairing appears to hold, respectively does not appear to hold. Generally, it seems to be easier to give sufficient conditions under which conjugate pairing does *not* hold: one example is a three-dimensional periodic Lorentz gas under electric and magnetic fields for which there is, or is not, conjugate pairing depending on the specific direction of the two fields [Dol00]. Another generic class of counterexamples to conjugate pairing is provided by systems that are thermostated at the boundaries [Pos88,Del97a,Wag00]. The latter models indicate that conjugate pairing is intimately related to the thermostat acting homogeneously and ‘democratically’ on all particles in the bulk of a system [Mor98,Eva00], whereas inhomogeneous thermostating at the boundaries prevents the Lyapunov exponents to come in conjugate pairs. In Chapter VII we will more explicitly discuss counterexamples of the latter type.

3. Fractal attractors characterizing nonequilibrium steady states

How does it fit together that *time-reversible* microscopic equations of motion yield *irreversible* macroscopic transport in a NSS? As was first discussed by Hoover et al. [Hol87,Mor87a] and by Morriss [Mor87b], for this type of driven thermostated systems reversibility and irreversibility are intimately linked to each other by the existence of a *fractal attractor* in phase space; see Refs. [Mor87b,Mor89b,Eva90b,Pet94] for a sheared two-particle system, Refs. [Pos87,Pos88,Mor89a,Pos89,Hoo94,Del97a,Wag00] for many-particle systems under various nonequilibrium conditions, Refs. [Mor87a,Hoo88a,Hoo89b,Van92,Hoo92,Che93a,Che93b,Lue93,Llo94,Llo95] [Del95a,Det96a,Det97c,Mor98,Hoo98c,Kla00b,Rat00b,Rat00a,Rat02] for the driven periodic Lorentz gas and Refs. [Hol87,Kus90,Hoo91,Tel96,Pos97,Pos98,Gil99a,Gil99b,Hoo99,Tel00,Vol02] for related models.¹⁸

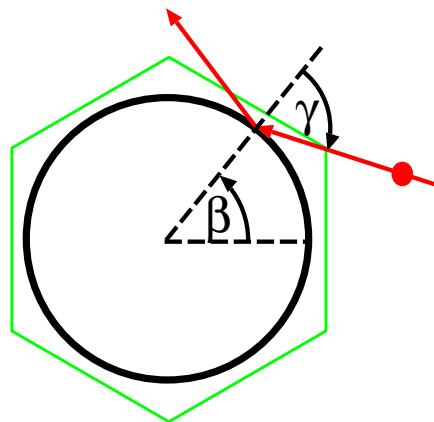


FIG. 4. Phase space coordinates describing the collision of a point particle with a disk in case of the two-dimensional periodic Lorentz gas. β denotes the position of the colliding particle on the circumference of the disk, whereas the impact angle γ is related to the direction of the velocity of the moving particle before the collision.

We now outline characteristic features of the attractor of the driven periodic Lorentz gas. For convenience the temperature of the thermostat is fixed at $T = 1$. In order to simplify the analysis a Poincaré surface of section is considered. That is, we introduce a further constraint in position space by representing the dynamics in terms of the phase space coordinates at a collision with a disk only. These collisions are defined by the position on the

¹⁸Here we are using the term *attractor* according to the operational definition of Eckmann and Ruelle [Eck85]: Let there be points in phase space generated by the equations of motion of a dynamical system. The attractor is the set on which these points accumulate for large times. For more rigorous mathematical definitions see, e.g., Refs. [Eck85,Gas98a,Guc90,Dev89]. Sometimes the additional term *strange* is employed to further characterize attractors [Rue71]. However, its use appears to be quite ambiguous in the literature, partly indicating the existence of a chaotic dynamics on the attracting set [Bec93,Sch89,Eck85,Lev89], partly being synonymous for the attractor exhibiting a fractal structure [Ott93,Gre84]. Hence, here we avoid this denotation.

circumference of the disk according to the angle β and by the impact angle γ related to the direction of the velocity of the moving particle, see Fig. 4. The set $(\beta, \sin \gamma)$ forms the *Birkhoff coordinates* of a particle billiard [Gas98a]. A convenient property of the Birkhoff coordinates is that in the Hamiltonian case at field strength $\varepsilon = 0$ the invariant probability density $\rho(\beta, \sin \gamma)$ associated with these coordinates is simply uniform in the whole accessible phase space. In contrast to that, Fig. 5 shows that in case of dissipation generated by an electric field and counterbalanced by a Gaussian thermostat the phase space density contracts onto a complicated fractal-looking object. Numerical analysis provides evidence that the attractor shown in Fig. 5 is *multifractal* [Ott93,Bec93,Lev89]: Although the two-dimensional phase space spanned by the Birkhoff coordinates is fully covered for small enough field strength yielding a box-counting dimension of two in computer simulations, the higher-order Renyi dimensions such as the information dimension and the correlation dimension are non-integer and slightly smaller than two indicating an inhomogeneous fractal folding of the phase space [Hoo89b,Det96a,Det00a].

However, note that here we are discussing the attractor in the reduced phase space defined by the Poincaré surface of section only. As far as the whole accessible phase space corresponding to the three independent phase space variables of the model is concerned there is a proof that the Hausdorff dimension of this fractal set is less than three and identical to the information dimension for non-zero but small enough field strength [Che93a,Che93b], which appears to be consistent with computer simulation results [Del95a].

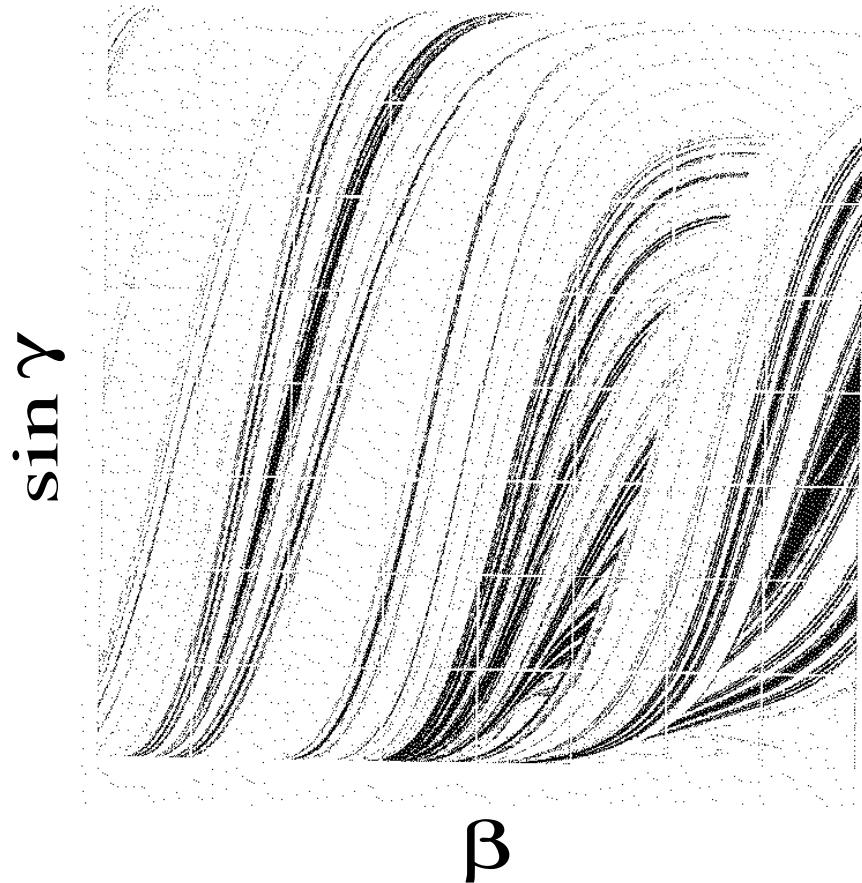


FIG. 5. Attractor for the Gaussian thermostated periodic Lorentz gas driven by an electric field of strength $\varepsilon = 1.5$ which, here, is parallel to the y -axis. The temperature is $T = 1$, β and $\sin \gamma$ are defined in Fig. 4. The figure, originally being a 1m-square, is from Ref. [Hoo89b]. For related results see Refs. [Mor87a,Hoo88a,Del95a,Hoo99].

The basic structure of the attractor shown in Fig. 5 can roughly be understood as follows: points in phase space with an impact angle of $\gamma = \pm\pi/2$ are reminiscent of *tangent collisions* where a moving particle just passes a disk. These points are due to the hard disk geometry and yield discontinuities in the equations of motion which separate regions in

phase space corresponding to different types of trajectories.¹⁹ Calculating higher iterates of these lines of discontinuity from the equations of motion yields complicated boundaries in phase space which match to the structures depicted in Fig. 5, see Refs. [Gas96,Gas98a] for the field-free Lorentz gas and Refs. [Mor87a,Hoo88a,Bon00] for the driven case. We remark that this procedure is intimately related to the construction of *Markov partitions* for the periodic Lorentz gas [Bun80,Bun81,Bun91,Che99]. Note that the topology of these structures changes under parameter variation, which has direct consequences for physical quantities such as the electrical conductivity of the system, as we will discuss in the following section.

The bifurcation diagram Fig. 6 indicates how the attractor changes by increasing the field strength ε [Mor87a,Hoo89b,Llo94,Llo95,Det96a,Mor98]. Here we show results for the angle θ which is the angle between the horizontal x -axis and the velocity of the moving particle after the collision. Consequently, θ is a simple function of the coordinate γ . Results for β and γ are analogous. This figure reveals a complicated bifurcation scenario: By increasing the field strength the attractor first experiences a *crisis* [Ott93] at which it suddenly collapses onto a subset in phase space [Llo94,Llo95,Det96a,Mor98]. For higher values of the field strength there are Feigenbaum-like bifurcations showing a complicated interplay between periodic windows and chaotic parameter regions. Around $\varepsilon = 2.4$ there is even an example of an elliptic fixed point in phase space.

Note that for small enough field strength, that is, before the first crisis occurs, the system is ergodic, see Refs. [Mor87a,Hoo89b,Llo94,Llo95,Det96a,Mor98] for numerical explorations and Refs. [Che93a,Che93b] for a proof. In the course of the bifurcations the system exhibits a complex transition scenario from ergodic and chaotic to non-ergodic and non-chaotic behavior. For high enough field strength the attractor eventually collapses onto a single periodic orbit. This orbit is such that a particle moves parallel to the field during a free flight, whereas at a collision it “creeps” along the circumference of a disk [Mor87a,Llo94,Llo95].

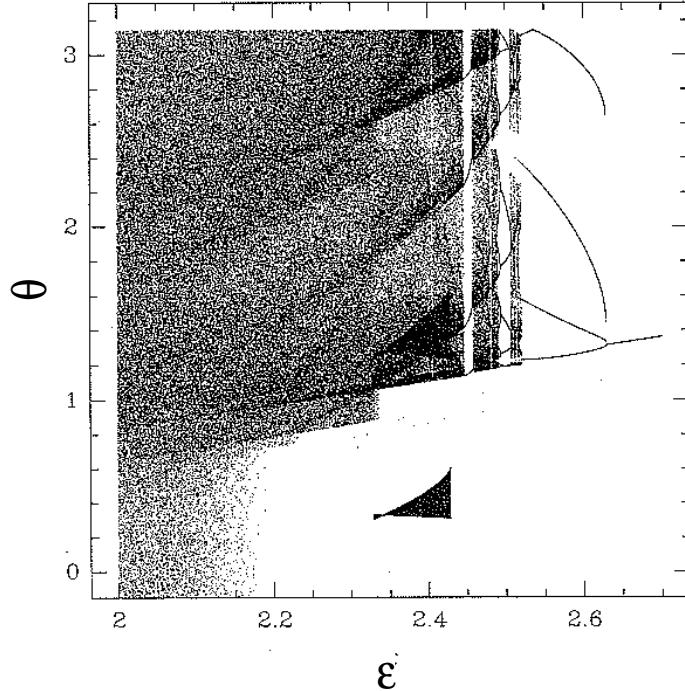


FIG. 6. Bifurcation diagram for the Gaussian thermostated periodic Lorentz gas driven by an electric field of strength ε which, here, is again parallel to the x -axis. θ is the angle between the x -axis and the velocity of the moving particle after the collision and is a simple function of γ as defined in Fig. 4. The temperature is set to $T = 1$. The figure is from Refs. [Llo94,Llo95,Mor98].

¹⁹With different types of trajectories we mean that trajectories of different regions hit different scatterers in the spatially extended periodic Lorentz gas, as can be quantitatively assessed in terms of a symbolic dynamics by assigning different symbols to different scatterers, see, e.g., Refs. [Llo94,Llo95,Gas96,Gas98a,Mor98] for further details.

For Gaussian-type thermostated dynamical systems the existence of multifractal attractors in respective Poincaré sections appears to be typical. This applies not only to a single-particle dynamics but also to interacting many-particle systems under general nonequilibrium conditions, see the long list of references cited at the beginning of this section for some examples. The fractality also survives in chaotic dynamical systems where the single particles interact with each other via smooth potentials [Pos87,Pos88,Pos89,Mor89a,Pos97,Hoo97] and in systems that are thermostated by a Stokes friction coefficient [Hoo92] or by some constant restitution coefficient at the collisions with a scatterer [Lue93]. Important questions are whether the existence of fractal attractors is a universal property of NSS in chaotic dynamical systems connected to thermal reservoirs, irrespective of the specific thermostat used, and to which extent the structure of the attractor depends on the specific type of thermostat.

4. Electrical conductivity and linear response for the Gaussian thermostated driven periodic Lorentz gas

In the final part of this chapter we focus on the transport properties of the Gaussian thermostated driven periodic Lorentz gas by studying the electrical conductivity $\sigma(\varepsilon)$ introduced in Eq. (32). Here we only discuss the ergodic regime of the model at field strengths $\varepsilon \ll 2$ for which $\sigma(\varepsilon)$ is uniquely defined. In this case it can be obtained from computer simulations in form of the time average over the velocity of a single particle sampled from a long trajectory. If the system is non-ergodic the situation is more complicated, since the values for the conductivity then depend on the choice of initial conditions in phase space. Results for $\sigma(\varepsilon)$ in the ergodic regime calculated from computer simulations [Llo95] are shown in Fig. 7. Related results have been obtained, also from simulations, in Refs. [Mor87a,Del95a,Bon00,Det00a]; for calculations based on periodic orbits see Refs. [Van92,Det97b], for the conductivity of a driven Lorentz gas thermostated by a Stokes friction coefficient see Ref. [Hoo92], and for conduction in a modified many-particle Lorentz gas see Refs. [Bar93,Bon97,Bon02].

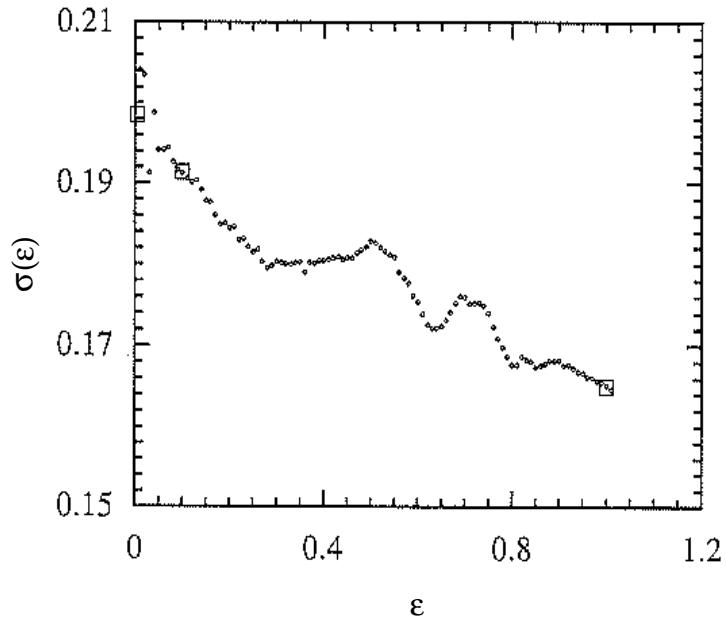


FIG. 7. Electrical conductivity $\sigma(\varepsilon)$ for the Gaussian thermostated periodic Lorentz gas driven by an electric field of strength ε which is parallel to the x -axis. The temperature is again $T = 1$. The small diamonds are data points computed from higher precision simulations, see Ref. [Llo95] for further details which also contains the original figure. Note the nonlinear response of this quantity and the irregular structure on fine scales.

Two aspects are remarkable in this figure: first of all, the validity of Ohm's law implies that the field-dependent conductivity is simply constant, $\sigma(\varepsilon) \equiv const.$ However, here this quantity clearly decreases on average thus indicating that, for the range of field strengths shown in the figure, the response is already in the nonlinear regime. Indeed, even for the smallest values of the field strength which are accessible to simulations no linear response be-

havior is visible in this figure. These results [Llo95] are in agreement with simulations performed by other authors [Mor87a,Del95a,Bon00,Det00a]. On the other hand, in the limit of $\varepsilon \rightarrow 0$ the conductivity appears to converge to the correct value of the diffusion coefficient obtained from the Einstein formula²⁰

$$D/T = \sigma(\varepsilon) \quad (\varepsilon \rightarrow 0) \quad , \quad (34)$$

which is $D \simeq 0.196$ for $T = 1$ [Mac83,Bar93,Gas95a,Mor94,Del95a,Bon00,Kla00a]. This numerically corroborates the analytical proof of the Einstein relation presented in Refs. [Che93a,Che93b]. For sake of completeness let us remark that the conductivity also depends on the density of scatterers. As expected, for higher densities the response appears to be getting more linear in the regime of field strengths shown in Fig. 7 [Del95a]. However, to decide about linearity or nonlinearity is still very ambiguous, since this depends on the scale according to which the results are plotted; see also Fig. 4 in Ref. [Det00a].

A second fact makes the situation even more complicated, namely the existence of irregularities in the conductivity as a function of the field strength in form of non-monotonicities on fine scales, as was first reported in Ref. [Mor87a]. The existence of such irregularities has also been verified by cycle expansion calculations for higher values of the field strength [Det97b] and by other computer simulations [Llo95,Del95a,Bon00], hence they are not artifacts representing numerical imprecisions. Indeed, this phenomenon extends the discussion of irregular and fractal transport coefficients outlined in the introduction [Kla95,Kla96,Kla99a,Gas98c,Har01,Gro02,Kor02] to the case of thermostated systems: by using Birkhoff coordinates the periodic Lorentz gas can be linked to maps having the same properties as the ones exhibiting fractal transport coefficients [Gas96,Gas98a,Gil99b,Gas98c,Tel00,Vol02]. It was thus early conjectured that the field-dependent conductivity of the driven Lorentz gas too exhibits fractal properties [Kla95,Kla96,Kla99a]. For one-dimensional maps with broken symmetry yielding drift-dependent currents it was shown that the conductivity is typically²¹ a nonlinear fractal function of control parameters [Gro02,Gil03]. Similar results were obtained numerically for the parameter-dependent diffusion coefficient in the field-free periodic Lorentz gas [Kla00a,Kla02c] and in related billiards of Lorentz-gas type [Har02]. However, to rigorously prove the existence of irregular structures in transport coefficients is generally a hard task, even for the most simple systems [Gro02], as is exemplified by a recent analysis for the driven Lorentz gas that was not conclusive in this respect [Bon00].

Apart from these numerical assessments of the Lorentz gas conductivity there are seminal mathematical results proving Ohm's law for this model [Che93a,Che93b]. However, this proof does not yield any precise upper bound for the validity of the range of linear response and may thus rather be considered as an existence proof. Indeed, simple heuristic arguments quantifying such bounds as discussed in Refs. [Dor99,Che93b] lead to wrong values for the driven periodic Lorentz gas in comparison to simulation results [Rat00b]. According to these mathematical and numerical analyses one may conclude that a regime of linear response exists in the driven periodic Lorentz gas which, however, is so small in the field strength that, up to now, it could not properly be detected in computer simulations. Even then, an open problem is the possible existence of fractal-like irregularities on fine scales, which for the driven Lorentz gas one may expect to persist as well in the limit of $\varepsilon \rightarrow 0$ [Gro02]. If this is the case Ohm's law may strictly speaking only hold with respect to performing a suitable coarse graining for the conductivity over small but finite subintervals of the field strength.

These problems strongly remind of the famous van Kampen objections against linear response theory [vK71]. It is not our goal here to give a full account of the debate around van Kampen's arguments. For that we may refer, e.g., to Refs. [Mor89c,Eva90b,Kub92,Che93b], to the nice outline in Ref. [Dor99] and to further references therein. Instead, we will highlight certain points that we believe are important for an understanding of the interplay between chaos and transport in the driven periodic Lorentz gas.

Van Kampen criticizes derivations of the laws of linear response that assume microscopic linearity in the equations of motion. By taking this assumption serious he arrives at a simple estimate for the range of validity of linear response which is $10^{-18}V/cm$ for electrons in a conductor.²² Van Kampen uses this unrealistically small value to illustrate

²⁰This equation is easily obtained from the Einstein relation Eq. (3) if an external electric field ε is added to the (one-dimensional) Langevin equation Eq. (1). In a NSS the average over the time derivative of the velocity on the left hand side of Eq. (1) must be zero and the average over the noise on the right hand side is by definition also zero, hence $E - \alpha < v > = 0$. By using Eq. (32) one arrives at $\sigma = 1/\alpha$ [Rei65,Pat88]. Note that for the Gaussian thermostated driven Lorentz gas Eqs. (23), (26) the validity of these relations is not obvious.

²¹i.e., for all control parameters except of Lebesgue measure zero

²²We remark that in Ref. [Bon00] a number for the range of validity has been given for the driven periodic Lorentz gas, "possibly as small as of 10^{-20} ", whose order of magnitude is close to the original estimate by van Kampen [vK71], however, without indicating how this value was calculated for this specific system.

his point that *linearity of the microscopic motion is entirely different from macroscopic linearity*. In other words, the question is how to reconcile the ubiquitous microscopic nonlinearity in the equations of motion of a dynamical system with the macroscopic linearity in the response of the same system. According to van Kampen *it is the randomization of the microscopic variables that enables one to eliminate them from the macroscopic picture*, whereas *in linear response theory the previous history is not forgotten through randomization, but ignored through linearization*. Curiously enough, van Kampen discusses just the Galton board under external forces as an example. By formally solving the Boltzmann equation that is based on Boltzmann's *molecular chaos* assumption he concludes that *the nonlinear deviations of the microscopic motions somehow combine to produce a linear macroscopic response*; see also Refs. [Che93b,Coh98,Kla00a] on discussions of that point.

To us, the existence proof of linear response for the driven periodic Lorentz gas given in Refs. [Che93a,Che93b] exemplifies how to reconcile macroscopic linearity with microscopic nonlinearity. On the other hand, results from computer simulations and related work [Mor87a,Llo95,Del95a,Det97b,Bon00] still point back to van Kampen's first objection how to quantitatively identify the regime of validity of linear response. Thus, the driven periodic Lorentz gas appears to provide a good illustration for the difficulty formulated by van Kampen that both the existence and the size of the regime of linear response may not be trivially guaranteed in a nonlinear dynamical system; see also Ref. [Gro02] for another example which is even more drastic but also more abstract than the Lorentz gas. A proper theoretical approach thus needs to take into account that, for microscopic chaotic dynamics, the macroscopic response of the system may very sensitively depend on the special character of the system. However, let us emphasize that the periodic Lorentz gas shares specific properties such as being low-dimensional and spatially periodic, which may not be considered to be typical for gases or fluids that are generally composed of many interacting particles. In random Lorentz gases, or in systems with more degrees of freedom, there is no evidence that the response exhibits problems of the type as described by van Kampen.

C. Summary

1. Using the mixing and chaotic periodic Lorentz gas as a simple model system saves us from adding noise in order to generate Brownian motion-like trajectories of a moving particle. This model thus provides an alternative to analyzing the interplay between subsystems and thermal reservoirs by means of stochastic Langevin equations. By furthermore making the friction coefficient velocity-dependent, under the constraint that the total kinetic energy of the system is constant at any time step, we arrive at the formulation of the *Gaussian thermostat* for the periodic Lorentz gas driven by an external electric field. Surprisingly, this combination of subsystem plus modeling of a thermal reservoir is still deterministic and time-reversible. It is also non-Hamiltonian reflecting that the resulting dynamical system is dissipative. The Gaussian thermostat is an example of a thermal reservoir that instantaneously acts in the bulk of a dynamical system.
2. For Gaussian thermostated dynamical systems in nonequilibrium situations there is an identity between the absolute value of the rate of phase space contraction and thermodynamic entropy production in terms of the Clausius entropy, respectively in terms of Joule's heat, by applying an external electric field. This identity represents a crucial link between dynamical systems quantities related to phase space contraction and thermodynamic quantities related to irreversible entropy production.
3. As a consequence of this identity the electrical conductivity is a simple function of the sum of Lyapunov exponents of the dynamical system, which is known as the *Lyapunov sum rule*. Similar formulas hold for other transport coefficients. Gaussian thermostated dynamical systems with more degrees of freedom, such as interacting many-particle systems, may furthermore exhibit a specific symmetry in the spectrum of Lyapunov exponents, which enables to split the spectrum into *conjugate pairs* of exponents all summing up to the same value. If conjugate pairs exist the Lyapunov sum rule can be drastically simplified. However, a necessary condition for this symmetry appears to be that the thermostat acts in the bulk of the system, whereas for boundary thermostats there are no such conjugate pairs. And even for bulk thermostats the precise conditions under which conjugate pairing holds are not perfectly clear and under active discussion.
4. Gaussian thermostated dynamical systems are characterized by the existence of *multifractal attractors* in the Poincaré sections of the phase space. For the Gaussian thermostated driven periodic Lorentz gas the fractal structure of the attractor is particularly determined by sequences of tangent collisions reflecting strong dynamical correlations. Under variation of the external electric field strength the topology of the attractor changes exhibiting a complex bifurcation scenario.

- Computer simulations yield that the electrical conductivity of this model is a nonlinear function of the electric field strength, which furthermore displays irregularities on fine scales that might be of a fractal origin. Ohms law is proven to hold for sufficiently small field strengths which supposedly were not yet accessible to computer simulations. The problem of detecting the regime of linear response reminds to some of van Kampen's objections against the validity of linear response in chaotic dynamical systems.

IV. THE NOSÉ-HOOVER THERMOSTAT

We construct and analyse a second fundamental form of deterministic and time-reversible thermal reservoirs known as the *Nosé-Hoover thermostat*. To motivate this scheme we need a Liouville equation that also holds for dissipative dynamical systems, which we introduce at the beginning of this chapter. We then focus on the chaos and transport properties of the Nosé-Hoover thermostated driven periodic Lorentz gas by characterizing the associated NSS. For this purpose we first check whether there holds an identity between the average phase space contraction rate and thermodynamic entropy production as it was obtained for the Gaussian thermostat. We then discuss computer simulation results for the attractor and for the electrical conductivity of the Nosé-Hoover driven periodic Lorentz gas by comparing them to their Gaussian counterparts. Finally, we briefly elaborate on subtleties resulting from the construction of the Nosé-Hoover thermostat, and we outline how this scheme can be generalized leading to a variety of additional, similar thermal reservoirs.

A. The Liouville equation for dissipative dynamical systems

Here we particularly follow the presentations of Refs. [Eva90b,Dor99]. For sake of simplicity we shall formally restrict ourselves to the case of a one-particle system such as the Lorentz gas. Let the position \mathbf{r} and the velocity \mathbf{v} of the point particle be defined by some equations of motion. We wish to consider an ensemble of particles moving in the same dynamical system. That is, we take a large collection of points in the accessible phase space of the system, which in general may be restricted by (geometric) boundary conditions, cp. also to Section II.C for related definitions. Let $\rho \equiv \rho(t, \mathbf{r}, \mathbf{v})$ be the distribution function, or probability density, associated with the ensemble of moving particles. It is the number of points of the ensemble which one can find in the phase space volume element $d\mathbf{r}d\mathbf{v}$ centered around the position (\mathbf{r}, \mathbf{v}) at time t divided by the size of this volume element and by the total number of points N of the ensemble. By integrating over the whole accessible phase space this function is properly normalized to one. Let us consider the fraction $N(t)/N$, where $N \equiv N(0)$ is the number of ensemble members at time zero while $N(t)$ is the number of points at time t . The total change of this fraction of ensemble points in a volume element V with surface A in the phase space obeys the balance equation

$$\frac{d}{dt} \frac{N(t)}{N} = \int_V d\mathbf{r}d\mathbf{v} \frac{\partial \rho}{\partial t} + \int_A d\mathbf{A} \cdot (\mathbf{F}\rho) , \quad (35)$$

where $(\dot{\mathbf{r}}, \dot{\mathbf{v}})^* = \mathbf{F} \equiv \mathbf{F}(\mathbf{r}, \mathbf{v})$ stands for the flux given by the equations of motion of a dynamical system such as, e.g., Eqs. (23), and $*$ denotes the transpose. The first integral stands for the source and the second one for the flux term. If we assume that once an ensemble of particles is chosen the number of points is conserved by the equations of motion, i.e., that there is no vanishing of points in phase space due to chemical reactions or related mechanisms, the left hand side must be zero at any instant of time. Applying Gauss' divergence theorem to the flux term, $\int_A d\mathbf{A} \cdot (\mathbf{F}\rho) = \int_V d\mathbf{r}d\mathbf{v} \nabla \cdot (\mathbf{F}\rho)$ with $\nabla := (\partial \mathbf{r}/\partial t, \partial \mathbf{v}/\partial t)^*$, enables us to combine both integrals of Eq. (35) leading to the differential formulation [Pat88,Dor99,Eva90b]

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\mathbf{F}\rho) = 0 \quad (36)$$

or alternatively

$$\frac{d\rho}{dt} + \rho(\nabla \cdot \mathbf{F}) = 0 . \quad (37)$$

Note that the continuity equation Eq. (35) formulates only the conservation of the *number of points* in phase space. Hence, Eqs. (36), (37) are valid even if the dynamical system is not phase space *volume* preserving. In turn, for Hamiltonian dynamical systems it is $\nabla \cdot \mathbf{F} = 0$ and the well-known Liouville equation for volume-preserving dynamics is recovered [Rei65,Hua87,Pat88,Dor99],

$$\frac{d\rho}{dt} = 0 \quad . \quad (38)$$

This equation expresses the fact that according to Hamiltonian dynamics an ensemble of points moves like an incompressible fluid in phase space, which is often referred to as the *Liouville theorem* in the literature [Rei65,Hua87]. On this occasion some historical remarks are necessary. In his original work [Lio38] Liouville did not care at all about Hamiltonian dynamics. He just started from the equations of motion for an arbitrary dynamical system and derived the evolution equation for its Jacobian determinant, from which Eq. (37) follows in a straightforward way. Hence, as pointed out by Andrey [And86],²³ Eq. (37) should rather simply be called “the Liouville equation”. However, in textbooks usually only Eq. (38) is derived and called “the Liouville equation” [Rei65,Hua87,Dor99], probably because Liouville’s work was mainly applied to Hamiltonian dynamics. Respectively, in the more specialized literature Eq. (37) is often denoted as “the generalized Liouville equation” [Ger73,Ste79,Ste80,And85,Ram86,Hoo99,Ram02]. In this review we will stick to the historically correct denotation and simply call Eq. (37) “the Liouville equation”.

Alternative derivations of the Liouville equation in its most general form can be found in Refs. [Ger73,Ste79,Ste80,And86,Ram02,Ser03], where we should highlight the seminal work of Gerlich [Ger73]. Recently Tuckerman et al. [Tuc97,MT99] derived a seemingly different (generalized) Liouville equation by claiming that Eq. (37) is not correct, see Refs. [Mun00,Tuc00] for summaries of this approach. The resulting controversy about the correct form of the Liouville equation [Hoo98a,Rei98,Tuc98b,Eva98,Tuc98a,MT99] was eventually resolved by Ramshaw [Ram02] starting from the observation that Eq. (37) is not covariant [Ram86]. However, covariance can be achieved by incorporating a respective coordinate transformation into the Liouville equation, which is generally a function of the metric. Along these lines the connection between Eq. (37) and the form of the Liouville equation considered in Refs. [Tuc97,Tuc98b,MT99] can be established. Applying this transformation both formulations turn out to be completely equivalent, however, for many purposes Eq. (37) appears to be the more convenient choice [Ram02].

The Gaussian thermostated driven Lorentz gas provides a simple example where the divergence in Eq. (37) does not disappear. It may thus be replaced by Eq. (28) leading to

$$\frac{\partial \rho}{\partial t} = \alpha \rho \quad . \quad (39)$$

By employing this equation the *Gibbs entropy production* for the Gaussian thermostated driven Lorentz gas can be computed right away, which furnishes an alternative derivation of the identity Eq. (30) between phase space contraction and thermodynamic entropy production [Dor99,Det00a]. This and further important implications of the Liouville equation concerning irreversibility and entropy production will be discussed in Section V.B.

We are now set up to introduce a second fundamental type of deterministic thermal reservoirs generalizing the Gaussian scheme. For this construction the Liouville equation Eq. (37) will be used as a convenient starting point.

B. Construction of the Nosé-Hoover thermostat

1. Heuristic derivation

As a crucial property of the Gaussian thermostated driven Lorentz gas the velocity distribution of the moving particle is intimately related to the microcanonical one, that is, the system is constrained onto an energy shell in phase space. Here we introduce a generalized thermostating scheme that, under certain conditions, enables to transform the velocities of a dynamical system onto a *canonical distribution* in thermal equilibrium. Our heuristic derivation follows the presentations in Refs. [Hoo85,Hoo91]; see also a respective short note in Ref. [Hol86] and a formal generalization of this argument in Refs. [Kus90,Bul90a]. We remark that quantum mechanical formulations of deterministic and time-reversible thermal reservoirs can be obtained along the same lines [Kus93,Men01,Kus02,Men03].

Let us start again from the driven Lorentz gas equations of motion Eqs. (23) that already exhibit a coupling with a thermal reservoir in form of the friction variable α . Let us now assume that α is not necessarily a simple analytical function of \mathbf{v} like the Gaussian thermostat Eq. (26), but that it is determined by some unknown differential equation instead. Formally, the equations of motion then read

$$(\dot{\mathbf{r}}, \dot{\mathbf{v}}, \dot{\alpha})^* = \mathbf{F}(\mathbf{r}, \mathbf{v}, \alpha) \quad , \quad (40)$$

²³see also the footnote on p.69 of Ref. [Gas98a] for a related brief historical note

and the generalized Liouville equation Eq. (37) can be written as

$$\frac{\partial \rho}{\partial t} + \dot{\mathbf{r}} \frac{\partial \rho}{\partial \mathbf{r}} + \dot{\mathbf{v}} \frac{\partial \rho}{\partial \mathbf{v}} + \dot{\alpha} \frac{\partial \rho}{\partial \alpha} + \rho \left[\frac{\partial \dot{\mathbf{r}}}{\partial \mathbf{r}} + \frac{\partial \dot{\mathbf{v}}}{\partial \mathbf{v}} + \frac{\partial \dot{\alpha}}{\partial \alpha} \right] = 0 \quad . \quad (41)$$

In contrast to the Gaussian thermostat, which was designed to keep the kinetic energy constant at any time step specifically in nonequilibrium, here our strategy is to define the thermostating mechanism first in thermal equilibrium. The goal is to come up with a dissipation term that transforms the velocity distribution of the subsystem onto the canonical one. In a second step we then create a nonequilibrium situation. Here we will check whether our thermostat is able to generate a NSS, and if so we will study what its precise properties are. In other words, our goal is to find a differential equation for α that is consistent with the existence of a canonical velocity distribution for an ensemble of subsystem particles. For this purpose we make the ansatz [Nos84a,Nos84b,Pos88,Pos89,Eva90b,Mor98,Hoo99]

$$\rho(t, \mathbf{r}, \mathbf{v}, \alpha) \equiv \text{const. } \exp \left[-\frac{v^2}{2T} - (\tau \alpha)^2 \right] \quad , \quad (42)$$

where both the distribution for the velocities of the subsystem and for the thermal reservoir variable α are assumed to be canonical, cp. to Eq. (21).²⁴ According to equipartitioning of energy T is identified as the temperature of the desired canonical distribution, and in thermal equilibrium this temperature should be identical to the temperature of the associated thermal reservoir. Furthermore, since α has a dimension of $1/\text{second}$ we needed to introduce the new quantity $\tau > 0$ with $[\tau] = s$ in order to make the exponent of the second term dimensionless.

We now combine Eq. (42) with the equations of motion for a single free particle, see Eqs. (23) with $\varepsilon = 0$. Feeding these equations as well as the ansatz for ρ into Eq. (37) yields for α the differential equation

$$\alpha \frac{v^2}{T} - \alpha \dot{\alpha} 2\tau^2 - 2\alpha + \frac{\partial \dot{\alpha}}{\partial \alpha} = 0 \quad . \quad (43)$$

This equation can be further simplified by *ad hoc* restricting to the case $\partial \dot{\alpha} / \partial \alpha = 0$. We then arrive at the simple solution

$$\dot{\alpha} = \frac{v^2 - 2T}{\tau^2 2T} \quad . \quad (44)$$

This differential equation for the thermostating variable α , together with the equations of motion Eqs. (23), defines the so-called *Nosé-Hoover thermostat* for the driven periodic Lorentz gas. The first version of such a thermostat transforming onto canonical distributions was developed by Nosé in 1984 [Nos84a,Nos84b]. His original derivation proceeded along different lines by starting from a generalized Hamiltonian formalism, see Section IV.C.2. Furthermore, it featured an at least for practical purposes spurious differential equation related to another reservoir variable, which was eliminated by Hoover [Hoo85]. This simplified version of the Nosé thermostat was coined the Nosé-Hoover thermostat [Eva85b]. In first explorations it was particularly applied to the harmonic oscillator, and the combined system was respectively called the *Nosé-Hoover oscillator* [Hoo85,Pos86,Hol86,Mar92b,Nos93,Hoo96a,Pos97,Hoo97,Lai03].

As for the Gaussian thermostat, the Nosé-Hoover scheme can be used *isokinetically* by only constraining the kinetic energy of particles, see above, or *isoenergetically* by constraining the total internal energy of soft particles consisting of kinetic plus potential energy [Mor98,Det00a,Ron02a]. It can also be adapted to drive interacting many-particle systems under nonequilibrium conditions into NSS [Nos84a,Nos84b,Pos88,Pos89,Eva90b,Hes96a,Mor98,Hoo99,Det00a,Mun00,Ron02a]. The results obtained from such simulations are typically well in agreement with predictions from irreversible thermodynamics and linear response theory [Eva90b,Sar98]. Hence, like the Gaussian modeling of a thermal reservoir the Nosé-Hoover scheme became a widely accepted useful tool for performing nonequilibrium molecular dynamics computer simulations not only of simple but also of more complex fluids such as polymer melts, liquid crystals and ferrofluids [Hes96a,Hes96b,Hes97], of proteins in water and of chemical processes in the condensed matter phase [Tuc00].

²⁴For an N -particle system with d degrees of freedom the exponent compiling the total energy of subsystem and thermal reservoir reads respectively $E_{total}/T = (\sum_i v_i^2/2 + NdT\tau^2\alpha^2/2)/T$ [Nos84a,Nos84b,Pos88,Pos89,Eva90b,Mor98,Hoo99].

2. Physics of this thermostat

First of all, like the equations of motion Eqs. (23), (26) of the Gaussian thermostated Lorentz gas the Nosé-Hoover counterparts Eqs. (23), (44) are as well deterministic and time-reversible but non-Hamiltonian. However, in contrast to the microcanonical Gaussian thermostat Nosé-Hoover was constructed for generating a canonical velocity distribution. More than Gaussian constraint dynamics, Nosé-Hoover thermostated systems may thus be considered as deterministic and time-reversible variants of Langevin dynamics, cp. Eqs. (23), (44) to Eq. (1).

For interacting many-particle systems the Nosé-Hoover thermostat conveniently works in thermal equilibrium [Nos84a,Eva85b,Pos89]. However, similar to the Gaussian thermostat this is not the case for the Lorentz gas without external fields, which is due to a malfunctioning of the friction coefficient related to the hard disk collisions [Rat00a]. Nevertheless we are safe in studying the driven Lorentz gas because, in analogy to the Gaussian thermostat, as soon as an electric field is added this problem disappears.

Following this comparison with Langevin dynamics one may inquire about the existence of a fluctuation-dissipation theorem such as Eq. (2) for equilibrium Nosé-Hoover dynamics. But as we already discussed in Section III.A, for dissipative deterministic dynamical systems such as the Gaussian or the Nosé-Hoover thermostated Lorentz gas there is no separation between stochastic forces and dissipation matching to the respective terms in the Langevin equation Eq. (1). Actually, for both deterministic thermostats the velocity-dependent friction coefficient is itself a fluctuating variable, in addition to the fact that the position space Lorentz gas dynamics is also nonlinear and fluctuating. Hence, a balance equation like Eq. (2) between a constant friction coefficient and stochastic forces cannot exist; however, for more general fluctuation-dissipation relations in case of deterministic dynamics see Ref. [Rue99b].

In order to better understand the action of the Nosé-Hoover frictional force let us look at the ensemble averaged version of Eq. (44),

$$\langle \dot{\alpha} \rangle = \frac{\langle v^2 \rangle - 2T}{\tau^2 2T} . \quad (45)$$

If the thermostat acts properly in equilibrium the average of the fluctuations of the thermostating variable α must be zero and consequently $\langle v^2 \rangle = 2T$ on the right hand side, which corresponds to equipartitioning of energy for a system with two degrees of freedom.²⁵ T thus serves as a control parameter representing the temperature of the thermal reservoir. Choosing some T the thermostat variable α acts accordingly in order to thermalize the subsystem onto the same temperature. Consequently, in contrast to the Gaussian thermostat the proper temperature is not attained instantaneously but with respect to an ensemble average over a canonical velocity distribution, as we stipulated with our ansatz Eq. (42). That is, for a Lorentz gas particle the kinetic energy is allowed to fluctuate in time around a mean value of $\langle v^2 \rangle / 2$.

As in case of the Gaussian thermostat, α supplemented by the respective dynamics for this variable represents both the coupling of the subsystem to the thermal reservoir as well as the action of the thermal reservoir itself. In a way, one may think of α as a dynamical variable on which all hypothetical degrees of freedom of the thermal reservoir are projected upon just for the purpose of dissipating energy from the subsystem. Along this line of reasoning τ may then be interpreted as the *reservoir response time* with respect to exchanging energy between the subsystem and the thermal reservoir. τ thus serves as another control parameter determining the efficiency of the interaction. Note that this control parameter does not exist for the Gaussian thermostat.

Let us look at the two limiting cases of Eq. (42) with respect to a variation of τ : For $\tau \rightarrow \infty$ obviously $\alpha \rightarrow const.$, and one recovers the familiar case of Newton's *irreversible* equations of motion with constant Stokes' friction. On the other hand, making τ smaller implies that there is a more immediate response of the reservoir to fluctuations of the kinetic energy in the subsystem. Consequently, in the limit of $\tau \rightarrow 0$ there must eventually be instantaneous control leading back to the constraint of keeping the kinetic energy constant at any time step as formulated by the Gaussian thermostat. This can be seen by moving τ^2 from the denominator on the right hand side of Eq. (44) to the left hand side and performing the limit $\tau \rightarrow 0$ enforcing $v^2 = 2T$.²⁶ For more detailed studies of how Nosé-Hoover dynamics depends on the value of the coupling constant τ see Refs. [Nos84b,Hoo85,Eva85b,Hol86,Nos91,Nos93,Hol95,Kus90].

²⁵Since here we do not have Gaussian constraints we may safely assume the existence of two degrees of freedom for the subsystem.

²⁶However, note that for a vanishing external field $\varepsilon = 0$ the friction coefficient of the Gaussian thermostat Eq. (26) is by default zero, at least for the driven periodic Lorentz gas. Without external forces the respective solution for Nosé-Hoover should therefore also go to zero for $\tau \rightarrow 0$. Thus, in detail the relation between the Gaussian and the Nosé-Hoover thermostat is more intricate, see also the discussion in Chapter VIII.

The Gaussian thermostat may furthermore be classified as a feedback mechanism that is *differential* in time, reflecting the existence of an explicit functional form for the velocity-dependent friction coefficient. The Nosé-Hoover equations can be seen as an *integral* version according to the formal solution of the differential equation for the friction variable

$$\alpha(t) = \alpha(0) + \int_0^t ds \dot{\alpha}(s) \quad (46)$$

with $\dot{\alpha}$ being determined by Eq. (44) [Hol86,Hol87,Hol95]. Interestingly, the existence of these two limiting cases shows up in the specific functional form of the velocity distribution under variation of τ : For $\tau \rightarrow 0$ and small enough field strength ε this function must evidently approach a microcanonical velocity distribution $\rho(v) \sim \delta(2E - v^2)$, whereas for $\tau \rightarrow \infty$ it yields a canonical one. Consequently, between these two limiting cases there must exist a superposition of the two different shapes in form of a *crater-like* velocity distribution with a dip at the place of the former maximum of the canonical distribution.

Indeed, right this transition is depicted in Fig. 8 where $\rho(v_x)$ for a Nosé-Hoover thermostated driven periodic Lorentz gas is represented for three different values of τ [Rat00a]; for related results concerning another, different dynamical system thermostated by Nosé-Hoover see Ref. [Nos91]. Note the symmetry breaking in Fig. 8 because of the external electric field, however, one clearly recognizes the approach towards a microcanonical distribution for $\tau \rightarrow 0$.²⁷ We will come back to a more explicit discussion of this interesting point in Chapter VIII, where it will be shown that crater-like velocity distribution functions that are very similar to the one discussed here play an important role for so-called active Brownian particles which are thought to model, among others, biological cell motility.

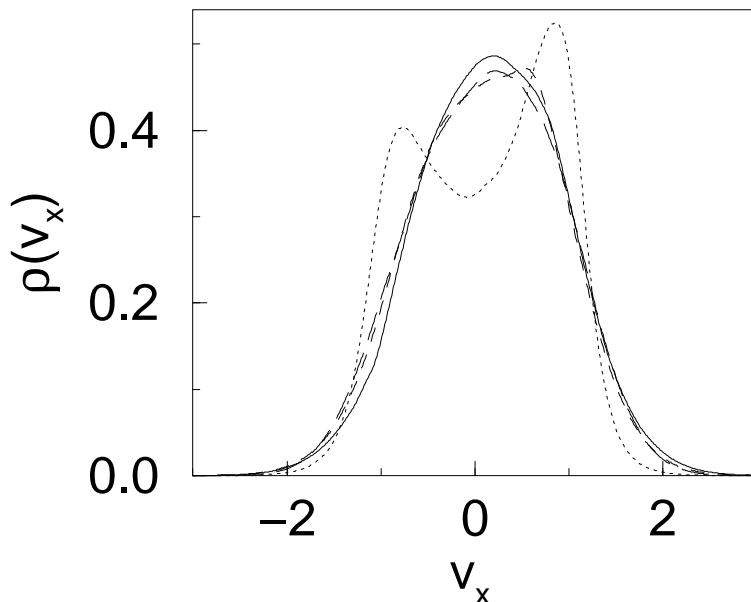


FIG. 8. Velocity distributions $\rho(v_x)$ for an ensemble of moving point particles in the thermostated driven periodic Lorentz gas for an electric field of strength $\varepsilon = 0.5$, which is parallel to the x -axis, at temperature $T = 0.60029$: Nosé-Hoover thermostat with a reponse time of the thermal reservoir of $\tau^2 = 0.01$ (dotted curve), $\tau^2 = 1$ (dashed curve), $\tau^2 = 1000$ (long dashed curve) in comparison to the application of the deterministic boundary thermostat (“thermostating by deterministic scattering”) discussed in Chapter VII (solid curve). Note the transition from a microcanonical-like to a canonical distribution under variation of τ . The figure is from Ref. [Rat00a].

²⁷Curiously, in case of *non-ergodic* Nosé-Hoover dynamics similar microcanonical-like and canonical-like distributions can be obtained with respect to different choices of initial conditions for the ensemble of particles, see the preprint of Ref. [Rat00a] for an example.

C. Properties of the Nosé-Hoover thermostat

1. Fundamental relations between chaos and transport

For the Gaussian thermostated driven Lorentz gas the crucial relation linking thermodynamics to dynamical systems theory was the identity Eq. (30) between the average phase space contraction rate and the thermodynamic entropy production in form of Joule's heat. Let us now check whether the Nosé-Hoover thermostat fulfills this identity as well. For this purpose we calculate the energy balance between subsystem and thermal reservoir [Pos88,Rat00a] by starting from the Hamiltonian for the combined system, see the exponent in Eq. (42),

$$H = v^2/2 + T\tau^2\alpha^2 \quad . \quad (47)$$

If the system is properly thermostated yielding a NSS, the average of the time derivative of the total energy must be zero, $\langle dH/dt \rangle = 0$. Differentiating Eq. (47) and replacing the derivatives by the equations of motion Eqs. (23), (44) yields

$$\frac{\langle \varepsilon \cdot \mathbf{v} \rangle}{T} = 2 \langle \alpha \rangle \quad (48)$$

The right hand side equals minus the average phase space contraction rate κ defined by Eq. (27), whereas the left hand side is obviously Joule's heat. We have thus corroborated the identity Eq. (30) for Nosé-Hoover dynamics.

Alternatively, in order to check for the identity one may start directly from the Nosé-Hoover equations of motion Eqs. (23), (44). Multiplying the differential equation for the velocity with \mathbf{v} and replacing the velocity squared on the right hand side by Eq. (44) one arrives at

$$\dot{\mathbf{v}} \cdot \mathbf{v} = \varepsilon \cdot \mathbf{v} - \alpha(\dot{\alpha}\tau^2 2T + 2T) \quad . \quad (49)$$

One may now collect all terms related to fluctuations on the left hand side by considering their statistical averages,

$$\langle \frac{d}{dt} \left(\frac{1}{2}v^2 + \tau^2 T \alpha^2 \right) \rangle = \langle \varepsilon \cdot \mathbf{v} - \alpha 2T \rangle \quad . \quad (50)$$

The left hand side is just identical to the average of the Hamiltonian Eq. (47) and must be zero in a NSS, see above, hence the right hand side yields again the identity. This derivation is useful if the Hamiltonian related to the thermostat is not known in advance, see Section VI.C for some examples.

Based on the identity Eq. (48) the Lyapunov sum rule can be derived in the same way as explained in Section III.B.2. For four nontrivial phase space variables it reads

$$\sigma(\varepsilon) = -\frac{T}{\varepsilon^2} \sum_{i=1}^4 \lambda_i(\varepsilon) \quad . \quad (51)$$

Hence, with respect to relations between chaos and transport the Nosé-Hoover thermostat belongs to precisely the same class of thermal reservoirs as the Gaussian one.

2. *Generalized Hamiltonian formalism for the Nosé-Hoover thermostat

A crucial feature of Hamiltonian systems is that the dynamics is phase space volume preserving, which follows from their symplectic structure [Mei92,Abr94]. On the other hand, as was shown for the Gaussian thermostat in Section III.B.1 and as we just verified for the Nosé-Hoover thermostat, the application of such deterministic thermostating mechanisms leads to an average phase space contraction in nonequilibrium. From that point of view it is surprising that for Gaussian and Nosé-Hoover dynamics a *generalized Lagrangian and Hamiltonian formalism* exists in which this dynamics is phase space volume preserving. Here we outline some main ideas of the Hamiltonian approach for the example of the isokinetic Nosé-Hoover thermostat.

Let us consider the very general case of a subsystem where a particle of unit mass moves under the influence of a potential $u(\mathbf{x})$. Let the microscopic dynamics of this particle be described by the phase space coordinates (\mathbf{r}, \mathbf{v}) . The dynamics of the thermal reservoir is modeled by only one degree of freedom in terms of the coordinates (r_0, v_0) . All these representations may be called *physical* coordinates, since (\mathbf{r}, \mathbf{v}) represents the actual position and the velocity of some particle. For the *decoupled* system the formal Hamiltonian is

$$H_0(\mathbf{r}, \mathbf{v}, r_0, v_0) = E(\mathbf{v}, v_0) + U(\mathbf{r}, r_0) , \quad (52)$$

where $E(\mathbf{v}, v_0) = m\mathbf{v}^2/2 + Qv_0^2/2$ stands for the kinetic energy of particle plus reservoir and $U(\mathbf{r}, r_0) = u(\mathbf{r}) + 2Tr_0$ for the potential energy of both systems. In formal analogy to the particle's kinetic energy, the new quantity Q is sometimes called the *mass* of the reservoir, and T is identified with the reservoir temperature.²⁸ The Hamiltonian equations of motion for the decoupled system then read

$$\begin{aligned}\dot{\mathbf{r}} &= \mathbf{v} \\ \dot{\mathbf{v}} &= -\frac{\partial u}{\partial \mathbf{r}} \\ \dot{r}_0 &= Qv_0 \\ \dot{v}_0 &= -2T .\end{aligned}\quad (53)$$

The problem is now two-fold: firstly, to find a Hamiltonian that generalizes Eq. (52) in suitably representing the *coupled* system, and secondly, to derive the Nosé-Hoover equations of motion, such as the special case Eqs. (23), (44) for the driven Lorentz gas, from this new Hamiltonian. In a slightly modified setting, this problem first appeared in Nosé's groundbreaking work [Nos84a,Nos84b] leading to the formulation of the so-called Nosé Hamiltonian. Here we follow a simplified approach as it was proposed later on in Refs. [Det97a,Cho98].

Since the Nosé-Hoover equations of motion are not Hamiltonian it is clear that a Hamiltonian formulation of this dynamics can only be achieved by choosing a new set of *generalized* coordinates, for which we may write (\mathbf{R}, \mathbf{V}) in case of the subsystem and (R_0, V_0) in case of the reservoir. Now we implement the so-called *exponential coupling ansatz* for the Hamiltonian in these generalized coordinates,

$$H(\mathbf{R}, \mathbf{V}, R_0, V_0) := e^{-R_0}E(\mathbf{V}, V_0) + e^{R_0}U(\mathbf{R}, R_0) . \quad (54)$$

These exponential prefactors define a *nonlinear, multiplicative coupling* between subsystem and thermal reservoir in generalized coordinates. Physically speaking, they suitably rescale the total energy of the system thus serving to keep the energy of the full system constant on average, whereas in nonequilibrium it would increase to infinity otherwise. The different signs of the exponents are adjusted to the different types of kinetic and potential energy. We can now derive Hamilton's equations of motion from this new Hamiltonian to

$$\begin{aligned}\dot{\mathbf{R}} &= e^{-R_0}m\mathbf{V} \\ \dot{\mathbf{V}} &= -e^{R_0}\frac{\partial u}{\partial \mathbf{R}} \\ \dot{R}_0 &= e^{-R_0}QV_0 \\ \dot{V}_0 &= 2(e^{-R_0}E(\mathbf{V}, V_0) - e^{R_0}T) .\end{aligned}\quad (55)$$

where we have imposed that $H(\mathbf{R}, \mathbf{V}, R_0, V_0) \equiv 0$. Matching the first two equations to the corresponding ones in physical coordinates Eqs. (53) suggests the following transformation between physical and generalized coordinates of the subsystem,

$$\begin{aligned}\mathbf{R} &= \mathbf{r} \\ \mathbf{V} &= e^{R_0}\mathbf{v} .\end{aligned}\quad (56)$$

Making the same choice for the reservoir coordinates,

$$\begin{aligned}R_0 &= r_0 \\ V_0 &= e^{R_0}v_0 ,\end{aligned}\quad (57)$$

we obtain a complete set of equations for transforming between physical and generalized coordinates. Identifying $Q \equiv 2T\tau^2$ and $\alpha \equiv v_0Q$ the Nosé-Hoover equations Eqs. (23), (44) for the driven Lorentz gas are precisely recovered from Eqs. (55). Let us emphasize at this point that the transformation between the different coordinates given by Eqs. (56), (57) is strictly *noncanonical* not preserving the phase space volume. Therefore, one should carefully

²⁸Strictly speaking the choice of the potential term for the reservoir, and fixing the number of degrees of freedom associated with it, is a bit more subtle [Cho98,Mor98].

distinguish between traditional Hamiltonian formulations of classical mechanics and the *generalized* Hamiltonian formalism outlined above.

The idea to use a generalized Hamiltonian formalism in order to define the action of a thermal reservoir was pioneered by Nosé [Nos84a,Nos84b] who constructed his thermostating mechanism along these lines. In Refs. [Nos91,Nos93,Hoo85,Eva85b,Pos86,Eva90b] this scheme was applied to different types of subsystems. Later on Dettmann and Morriss showed that there also exist generalized Hamiltonian formulations for the Gaussian isokinetic [Det96b] and isoenergetic [Det99a] thermostat, see Ref. [Hoo88a] for a pre-version of this approach. They also came up with a modified Nosé Hamiltonian leading more straightforwardly to the Nosé-Hoover equations than starting from Nosé's original formulation [Det97a,Hoo99], as is sketched in the derivation above. The generalized Lagrangian approach was outlined by Choquard in Ref. [Cho98], see also this reference as well as Refs. [Mor98,Det00a] for summaries concerning the subject of this section. We remark that the symplectic properties of these generalized Hamiltonians appear to be intimately related to the validity of the conjugate pairing rule discussed in Section III.B.2.

3. Attractors, bifurcation diagrams and electrical conductivities for the Nosé-Hoover thermostated driven periodic Lorentz gas

As we have shown in Sections III.B.1 and IV.C.1, both the Gaussian and the Nosé-Hoover thermostated driven Lorentz gas exhibit an identity between the average phase space contraction rate and thermodynamic entropy production. For the Nosé-Hoover case we now discuss further chaos and transport properties, which are the fractality of the corresponding attractor, the structure of the associated bifurcation diagram and the response to an electric field in terms of the field-dependent conductivity. Particularly, we elaborate on similarities and differences of these properties in comparison to the respective figures shown for the Gaussian thermostat. The computer simulation results for the Nosé-Hoover thermostated driven periodic Lorentz gas presented here are from Ref. [Rat00a].

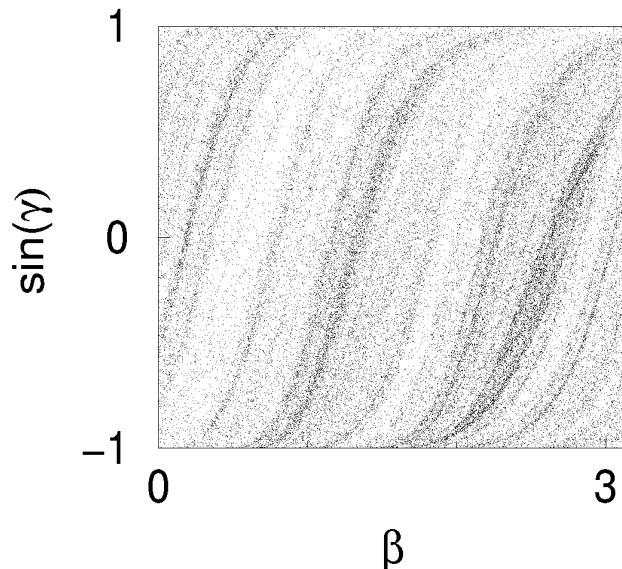


FIG. 9. Attractor for the Nosé-Hoover thermostated periodic Lorentz gas driven by an electric field of strength $\varepsilon = 1$ which is parallel to the x -axis. β and $\sin \gamma$ are the same as in Fig. 5 and are also defined in Fig. 4. The temperature is $T = 0.7740645$. The reservoir coupling parameter τ , see Eq. (44), has the value 0.1. The results are from Ref. [Rat00a].

Fig. 9 depicts a projection of the attractor of the Nosé-Hoover thermostated driven periodic Lorentz gas onto the phase space in Birkhoff coordinates.²⁹ Some repeated folding in phase space is clearly visible indicating that, as in

²⁹Note that, in contrast to the Gaussian thermostated driven periodic Lorentz gas, Fig. 9 does not represent a Poincaré surface of section: For Nosé-Hoover the kinetic energy is not kept constant but fluctuates, hence this plot is composed of points with different absolute values of the velocity of the colliding particle.

case of the Gaussian thermostat, most probably this attractor is again of a multifractal nature. However, for Nosé-Hoover yet no values for a (fractal) dimension quantitatively assessing this structure were computed.³⁰ By comparing this attractor to the one obtained from Gaussian thermostating Fig. 5 one realizes that the structure of both sets is essentially the same. This is not too surprising since both systems share the same geometry, and as we discussed in Section III.B.3 the main features of this structure are induced by the geometry of the scatterers. That the Nosé-Hoover thermostat attempts to transform the system onto a canonical distribution explains why the attractor related to the Nosé-Hoover thermostat appears to be a smoothed-out version of the Gaussian counterpart. These results suggest that the appearance of fractal attractors is also typical for Nosé-Hoover thermostated systems. Numerical computations of fractal dimensionality losses in many-particle systems thermostated by Nosé-Hoover confirm this statement [Hol87,Pos88,Pos89,Aok02,Kus02,Hoo02b,Pos03].

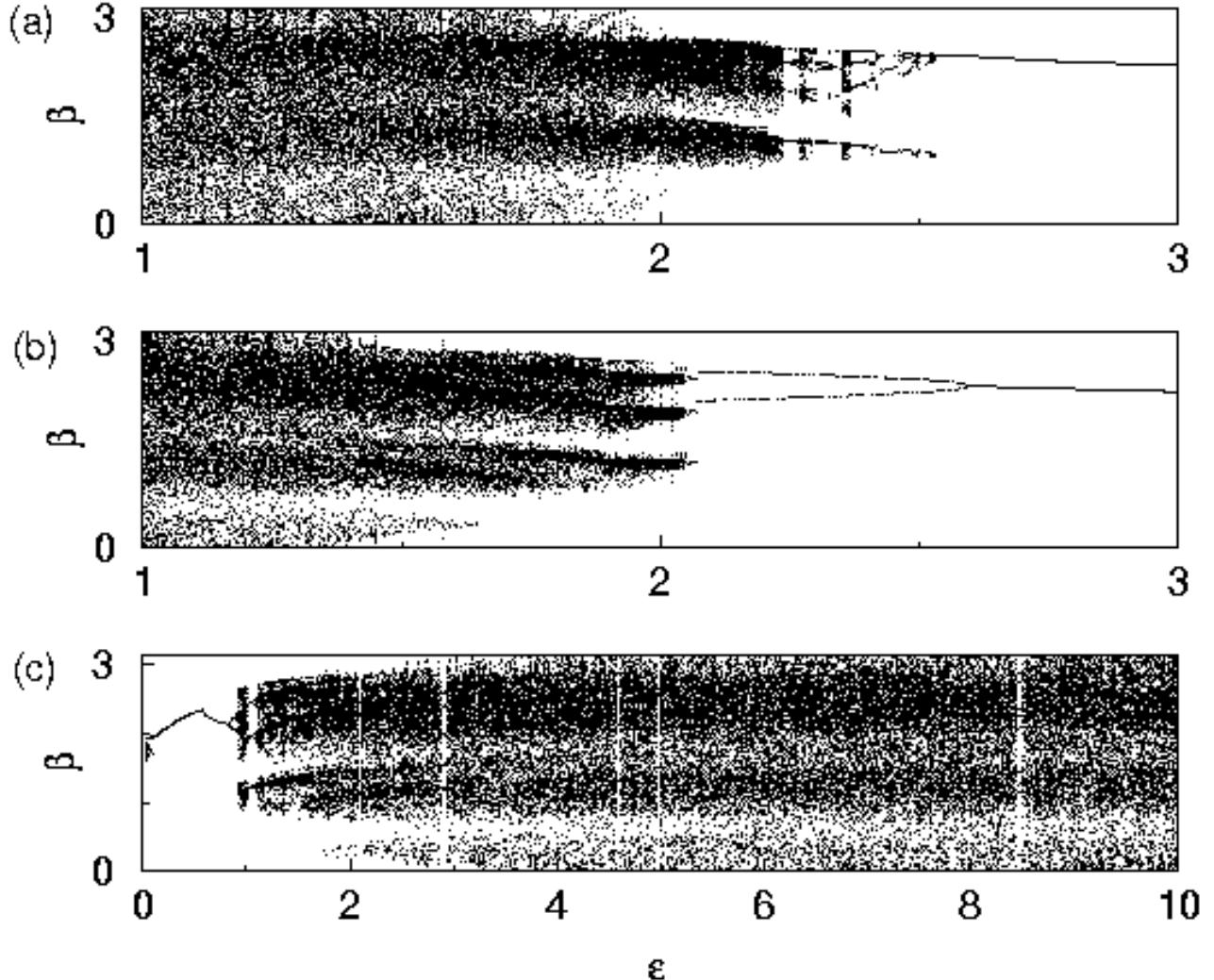


FIG. 10. Bifurcation diagrams for the Nosé-Hoover thermostated periodic Lorentz gas driven by an electric field of strength ϵ which is parallel to the x -axis. β is defined in Fig. 4. The temperature is fixed to $T = 0.5$ and the values of the reservoir coupling parameter τ , see Eq. (44), are: (a) $\tau = 0.1$, (b) $\tau \approx 31.6$ ($\tau^2 = 1000$) and (c) the dissipative limit of $\tau \rightarrow \infty$ corresponding to a constant friction coefficient α whose value was chosen to be 1. The figure is from Ref. [Rat00a].

Fig. 10 contains bifurcation diagrams for the Nosé-Hoover thermostated driven periodic Lorentz gas at three different values of the reservoir coupling constant τ , see Eq. (44). For quick response of the reservoir, $\tau \ll 1$, the attractor is

³⁰but see Section VII.D.2 for a very similar attractor for which the Kaplan-Yorke dimension was found to be fractal

phase space filling up to $\varepsilon < 2$, which is reminiscent of the results for the Gaussian thermostated Lorentz gas presented in Fig. 6. Note that Fig. 6 depicts the angle θ as a function of the field strength ε , whereas Fig. 10 displays the angle β , respectively. However, both bifurcation diagrams exhibit qualitatively the same behavior. This is in agreement with the discussion of Section III.B.2 where we argued that the Nosé-Hoover thermostat yields Gaussian constraint dynamics in the limit of $\tau \rightarrow 0$.

In agreement to a naive physical reasoning, by making the response time of the reservoir larger the attractor collapses onto periodic orbits at smaller field strengths than for smaller response times, see Fig. 10 (b). However, in detail the situation is much more intricate [Rat00a], as is already indicated by Fig. 10 (c) that displays the dissipative limit of $\tau \rightarrow \infty$. Here the bifurcation diagram depends on the value for the constant friction coefficient α . In any case, for all values studied numerically one observes a kind of inverted bifurcation scenario compared to the Gaussian thermostated model and to Figs. 10 (a) and (b) in that the attractor starts with periodic orbits and covers the whole accessible phase space only for higher field strengths [Rat00a]. Fig. 10 thus shows that for the Nosé-Hoover thermostated driven periodic Lorentz gas the specific structure of the fractal attractor sensitively depends on the choice of the reservoir coupling parameter τ ; see also Refs. [Nos84b,Hoo85,Eva85b,Hol86,Nos91,Nos93,Hol95,Kus90] for studies concerning the variation of τ in other systems and for the impact on dynamical systems properties.

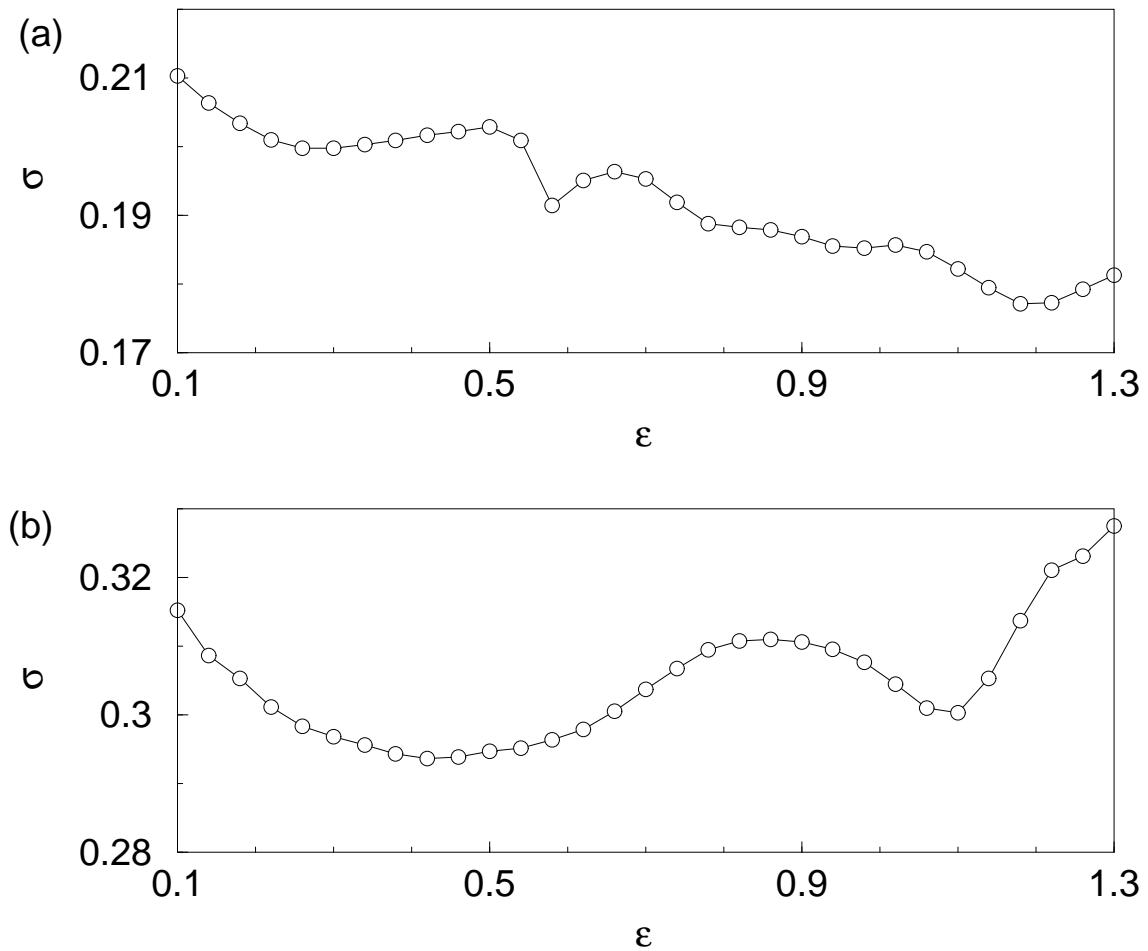


FIG. 11. Electrical conductivity $\sigma(\varepsilon)$ for the Nosé-Hoover thermostated periodic Lorentz gas driven by an electric field of strength ε which is parallel to the x -axis. The temperature is $T = 0.5$ and the values of the reservoir coupling parameter τ , see Eq. (44), are: (a) $\tau = 0.1$ and (b) $\tau \approx 31.6$ ($\tau^2 = 1000$). The numerical uncertainty of each point is less than the symbol size. The figure is from Ref. [Rat00a].

As one might suspect already with respect to these bifurcation diagrams, there is no unique result for the field-dependent electrical conductivity $\sigma(\varepsilon)$ at different values of the response time τ either, not even for small field strengths $\varepsilon \ll 2$. Fig. 11 presents computer simulation results for the two parameter values of τ studied in Figs. 10 (a) and (b). The conductivity for $\tau = 0.1$ looks like a smoothed-out version of the Gaussian thermostat conductivity

depicted in Fig. 7, whereas the curve at $\tau \simeq 31.6$ appears to be more stretched out along the ε -axis. In the latter case it is not even clear whether the conductivity is globally decreasing or increasing. There is little to say concerning the validity of the Einstein relation Eq. (34) in the limits of $\tau > 0$ and $\varepsilon \rightarrow 0$ as discussed for the Gaussian version in Section III.B.4, since the Nosé-Hoover thermostat does not work properly for the Lorentz gas in thermal equilibrium, see Section IV.B.2. Hence, the field-free diffusion coefficient cannot be computed independently.

That both field-dependent Nosé-Hoover conductivities are significantly less irregular than the Gaussian thermostat result of Fig. 7 may be understood with respect to the more “stochastic” nature of the Nosé-Hoover thermostat. According to its definition it modifies the billiard dynamics more profoundly than in case of the Gaussian constraint by transforming onto canonical velocity distributions, see again Fig. 8 for the probability densities at these parameters. Nevertheless, both conductivities still exhibit pronounced irregularities in form of non-monotonocities, and there are no indications for a regime of linear response, at least not in the numerically accessible region of $\varepsilon > 0.1$. In other words, even the Nosé-Hoover thermostat featuring a canonical velocity distribution does not lead to a more profound appearance of a regime representing Ohm’s law.

In summary, from a statistical mechanical point of view we have the rather unpleasant result that not only dynamical systems properties such as bifurcation diagrams but also transport properties such as the field-dependent electrical conductivity of the deterministically thermostated, driven periodic Lorentz gas strongly depend on details of the specific way of thermostating. However, as in case of the discussion of van Kampen’s criticism in Section III.B.4 one may speculate that this is rather a consequence of the small number of degrees of freedom and of the spatial periodicity of this model.

D. *Subtleties and generalizations of the Nosé-Hoover thermostat

1. Necessary conditions for Nosé-Hoover thermostating and generalizations of this scheme

As we briefly discussed in Sections III.A and IV.B.2, both the Gaussian and the Nosé-Hoover thermostat do not work properly for the periodic Lorentz gas without external fields: In this case the Gaussian thermostat is trivially non-existent, since the kinetic energy of the moving particle is conserved by definition anyway, whereas the Nosé-Hoover thermostat does not act appropriately because of the hard disk collisions. Controlling the two velocity variables *separately* by Nosé-Hoover eliminates this problem [Rat00a]. In any case, as outlined in the previous sections for both thermostats a small electric field resolves these intricacies leading to well-defined NSS. Apart from that, for interacting many-particle systems it was confirmed numerically that both the Gaussian [Hoo82,Eva83b,Pos88] and the Nosé-Hoover thermostat [Nos84a,Eva85b,Pos89] work correctly even in thermal equilibrium. These examples suggest that the thermostated subsystem must fulfill certain necessary conditions in order attain canonical velocity distributions.

In the literature this problem became well-known by studying both the *Nosé-Hoover oscillator*, which is a harmonic oscillator subject to a Nosé-Hoover thermostat, and a respectively thermalized particle moving in a double-well potential. Already in early computer simulations of the Nosé-Hoover oscillator it was observed that this system did not attain a canonical velocity distribution in thermal equilibrium [Hoo85,Pos86,Hol86]. This is due to the fact that the unperturbed harmonic oscillator is non-chaotic and perfectly integrable. Hence, under application of some thermal reservoir its regular phase space structure may just be getting deformed, and there is no reason why the resulting subsystem should become fully ergodic.

However, if such a previously regular subsystem is not driven to ergodic behavior by the action of some thermostat the whole phase space will not be sampled appropriately. As a consequence, the resulting velocity distribution may strongly depend on initial conditions and is typically not the canonical one [Hoo85,Pos86,Hol86,Kus90,Bul90a] [Ham90,Hoo91,Win92,Mar92b,L’H93,Nos93,Win95,Hoo96a,Hoo97,Mun00,Liu00,Hoo01,Ser01,Lai03]. The same applies to the Nosé-Hoover thermostated double-well potential [Kus90,L’H93,Win95,Bar03]. Jellinek and Berry [Jel88a,Jel89] and Kusnezov et al. [Kus90,Bul90a] thus emphasized that chaos and ergodic behavior are necessary conditions in order to thermalize a subsystem onto a canonical velocity distribution. This indicates that a thermostated subsystem should strictly speaking be mixing [Arn68,Sch89,Gas98a,Dor99] implying ergodicity and, under rather general conditions, also chaotic behavior [Dev89,Ban92].

These difficulties motivated the construction of a large variety of generalizations of the original Nosé-Hoover thermostat [Hoo89a,Kus90,Bul90a,Bul90b,Ham90,Hoo91,Win92,Mar92b,L’H93,Win95,Hoo96a,Pos97,Hoo97,Bon99,Mun00,Liu00] [Lai03,Bra00a,Bra00b,Hoo01,Ser01,Bar03]. The formal basis for these efforts was laid out again by Jellinek and Berry [Jel88a,Jel88b] and by Kusnezov et al. [Kus90,Bul90a]: Jellinek and Berry showed that there is the additional freedom of changing the *multiplicative* coupling between subsystem and thermal reservoir in generalized coordinates while

still being consistent with Nosé's basic idea of transforming onto canonical distributions.³¹ Kusnezov et al., in turn, pointed out that further *additive* contributions to Hamilton's equations of motion in generalized variables, see Eqs. (55), are possible, again without contradicting the existence of canonical velocity distributions. Both approaches will typically lead to thermostated equations of motion that are still time-reversible but more nonlinear than the ones corresponding to the original Nosé-Hoover scheme. Thus Nosé-Hoover represents just one choice of infinitely many for modeling a deterministic thermal reservoir transforming onto canonical distributions.

Starting from this important conclusion alternatives to Gaussian and Nosé-Hoover dynamics were explored by many authors. Their strategy was to improve the Nosé-Hoover scheme by constructing a thermostat that is able to conveniently thermalize the harmonic oscillator, or the double-well problem, onto a canonical velocity distribution in equilibrium. A straightforward generalization along the lines of Nosé-Hoover is the thermalization of higher even moments of the subsystem's velocity distribution onto the canonical ones by means of additional thermostating variables [Hoo89a,Jel89,Hoo96a,Pos97,Hoo97,Liu00]. Another formal option is to thermalize the position coordinates of a moving particle leading to the cubic coupling scheme [Kus90,Bul90a]. Enforcing the virial theorem, Hamilton used a linear scaling of the position coordinates [Ham90], which later on was combined with some multiplicative coupling [L'H93]. A thermalization of odd and even particle velocities, partly supplemented by using higher powers of the corresponding friction coefficients, was also explored and was argued to represent a deterministic, time-reversible analogue of the stochastic Langevin equation [Bul90b]. More recently, a directional thermostat called *twirler* stirring the angular momentum of a moving particle was introduced and applied in suitable combination with Gaussian and Nosé-Hoover thermostats [Hes02,Hes03].

Another scheme that became rather popular is the Nosé-Hoover chain thermostat [Mar92b,Tuc00] that couples the differential equation for the Nosé-Hoover friction coefficient additively to another Nosé-Hoover friction coefficient, and so on. However, this solution was assessed to be unstable out of equilibrium [Eva98,Bra00a] leading to another modification of it [Bra00a]. Some multiplicative extensions of Nosé-Hoover along the lines of Jellinek's formalism have been worked out by Winkler et al. [Win92,Win95] and became further amended in Ref. [Bra00b]. Another, in a way, multiplicative variant was discussed in Ref. [Ser01].

We finally mention the so-called Nosé-Poincaré method representing a scheme that is in-between the original approaches by Nosé and Nosé-Hoover. The resulting dynamics is identical to Nosé-Hoover, however, it is generated by symplectic equations of motion that enable the application of symplectic integration algorithms, which considerably increases the numerical precision [Bon99,Bar03]. A further extension of this approach allowing to model generalized types of Nosé-Hoover dynamics along these lines, which appears to share quite some similarities with Jellinek's ideas [Jel88a,Jel88b], was recently proposed in Ref. [Lai03].

It is not the purpose of this review to give a full account of the specific physical and numerical advantages and disadvantages of all these different thermostating schemes. Here we may refer, e.g., to Refs. [Jel88a,Hoo96a,Pos97,Hoo97,Bra00a] that partly review and criticize these more recent methods. Following Jellinek, Branka and Wojciechowski [Bra00b] particularly endeavored to systematically explore the numerical practicability and efficiency of these different classes of thermostats. They arrived at essentially ruling out many of the up to now existing solutions. Further, more physical constraints contradicting some of the methods mentioned above will be briefly summarized in the following section.

However, in our view one may even go so far to question the philosophy underlying most of these novel constructions in that a 'good' thermostat should, by all means, enforce a canonical velocity distribution even for regular dynamical systems such as the harmonic oscillator. The other way around, one may argue that the harmonic oscillator is rather unsuited to be properly thermalized at all just because of its inherent regularity. Correspondingly, a successful transformation of this dynamics onto a canonical velocity distribution indicates that the original dynamics of this system is profoundly destroyed according to the action of the thermal reservoir. This raises the question to which extent the resulting dynamics represents merely the action of the thermostat and whether anything is left at all of the original characteristics of the previously regular subsystem. Nevertheless, we suspect that for practical computational purposes it is still desirable to have a thermostat at hand which is capable to always create a canonical velocity distribution irrespective of the detailed properties of the original dynamical system to which it is applied.

This discussion clearly demonstrates that the world of deterministic and time-reversible thermostats does not only consist of Gaussian and Nosé-Hoover thermostats. Obviously, there exists a microcosmos of variants of them. This

³¹In more detail, starting from the Nosé Hamiltonian they showed that changing the scaling rules between the physical and the generalized variables, cp. to Eqs. (56), (57), plus possibly also changing a time scaling between physical and generalized time (that we did not discuss in Section IV.C.2) is not at variance with canonical velocity distributions being the solutions of the respective Liouville equation Eq. (37).

should be taken into account if one attempts to come to general conclusions concerning the second law of thermodynamics and the universality of chaotic and transport properties of NSS based on the analysis of Gaussian and Nosé-Hoover thermostats only.

2. Applying thermal reservoirs to nonequilibrium situations

In Section II.C we have argued that thermal reservoirs should generally be constructed in equilibrium situations. In this case the statistical ensembles are well-defined and the corresponding velocity distribution functions for subsystem and thermal reservoir are known exactly. After their definition in thermal equilibrium one may apply these reservoirs for thermalizing a subsystem under nonequilibrium constraints, by expecting that the respective thermostat still works sufficiently well such that a proper NSS is created. One may now learn something new about the NSS resulting for a particular subsystem by analyzing the corresponding nonequilibrium distribution functions as well as the associated chaos and transport properties, which are generally not known in advance.

However, first of all, it is not guaranteed that a thermal reservoir which properly acts in thermal equilibrium also functions in nonequilibrium by generating a NSS. Actually, it appears that most of the generalizations of the Nosé-Hoover thermostat listed above have only been tested in thermal equilibrium so far. Some of them have already been criticized for not working properly under nonequilibrium constraints [Eva98,Bra00a,Bra00b]. Apart from that, only a few studies of nonequilibrium situations are available for these generalized reservoirs [Pos97,Hoo97,Bra00a,Bra00b]. The same applies to the chaotic dynamical properties of subsystems connected to these different thermal reservoirs even in thermal equilibrium, see only Refs. [Kus90,Mar92b,Pos97,Hoo01] for results of some specific cases.

Secondly, a thermal reservoir should always remain in thermal equilibrium, even if the subsystem is under nonequilibrium constraints, and it should only control the temperature of the subsystem, or possibly respective higher moments of it. Consequently, a thermal reservoir should only act on the even moments of the velocity distribution of a subsystem. If a thermal reservoir were defined to also control odd moments of the velocity its action goes beyond simple temperature control and may change the dynamics of the subsystem profoundly. For example, in the driven periodic Lorentz gas the first moment of the velocity yields the current of the subsystem in nonequilibrium. Thus, a thermostat that constrains this quantity would simply pre-determine the current.³² In the same vein, a thermal reservoir acting onto position coordinates may pre-determine, or at least profoundly influence, the respective moments of the position coordinates hence affecting transport coefficients like diffusion and higher-order Burnett coefficients. Consequently, on the basis of physical grounds one may wish to constrain the action of thermal reservoirs to even velocity moments only. If one follows this argumentation, this already rules out schemes such as the ones presented in Refs. [Kus90,Bul90b,Bul90a,Ham90,L'H93].

In conclusion, all what one can demand is that a thermal reservoir properly acts in a thermal equilibrium situation by thermalizing a subsystem onto a pre-determined velocity distribution. In nonequilibrium the general requirement should be the existence of a NSS at a certain temperature, whose properties as resulting from the action of this thermal reservoir may then be studied respectively.

E. Summary

1. Starting from the conservation of the number of points in phase space we have derived the Liouville equation for dissipative dynamical systems. The Hamiltonian version of this Liouville equation, which typically appears in textbooks, is obtained from it under the additional assumption of conservation of phase space volume.
2. By employing the general form of the Liouville equation and by requiring that canonical distributions for the velocities of a subsystem and for a reservoir variable exist, we arrived at a simple differential equation determining the velocity-dependent friction coefficient. This equation defines the action of the *Nosé-Hoover thermostat*, supplemented by a respective friction term in the original equations of motion of the subsystem.

In complete analogy to the Gaussian thermostat, Nosé-Hoover thermostated equations of motion are deterministic and time-reversible but non-Hamiltonian. However, in contrast to the Gaussian reservoir the Nosé-Hoover

³²Note, however, that a thermal reservoir may be defined such that it is comoving with the current, in order to thermalize the subsystem onto the proper temperature in the comoving frame; see Refs. [Pos88,Sea98] and also the discussion of a thermostated shear flow in Section VII.E, respectively Refs. [Wag99,Wag00].

scheme, by construction, attempts to transform the subsystem velocities onto a canonical distribution in thermal equilibrium. Hence, it yields a dynamics that is more similar to Langevin's theory than the one resulting from the Gaussian constraint of constant energy. Another difference of the Nosé-Hoover thermostat compared to the Gaussian one is the appearance of an additional control parameter that may be interpreted as the response time of the thermal reservoir regarding its interaction with a subsystem. In case of infinitely slow response the Stokes friction coefficient is recovered, whereas for infinitesimally quick response the Gaussian constraint is approached. A variation of this control parameter changes the shapes of the corresponding velocity distributions that may accordingly be composed of superpositions of microcanonical and canonical densities.

3. The Nosé-Hoover thermostat belongs to the same class of deterministic and time-reversible thermal reservoirs as the Gaussian one as far as an identity between the average rate of phase space contraction and thermodynamic entropy production is concerned. Respectively, there is also an analogous relation between transport coefficients and Lyapunov exponents for Nosé-Hoover dynamics.

For both thermal reservoirs there exist generalized Hamiltonian and Lagrangian formulations. For the isokinetic Nosé-Hoover thermostat we have outlined how to derive the respective equations of motion from a Hamiltonian in generalized variables via non-canonical transformations.

Like the Gaussian thermostated driven periodic Lorentz gas, the Nosé-Hoover version is as well characterized by a fractal attractor of a similar type. The specific structure of this attractor depends on the value of the reservoir response time. For large enough response times the bifurcations displayed by this fractal attractor are typically very different from the ones observed for the Gaussian reservoir. The same applies to the field-dependent electrical conductivities in case of Nosé-Hoover, which still show irregularities on fine scales and no indication of linear response in the numerically accessible regime of the field strength.

4. Finally, we have summarized problems with Gaussian and particularly with Nosé-Hoover thermostats in equilibrium and nonequilibrium situations. For regular dynamical systems such as the harmonic oscillator or a particle moving in a double-well potential it is well-known that the standard Nosé-Hoover thermostat is not able to thermalize these systems onto canonical velocity distributions in thermal equilibrium. A necessary condition is that the thermostated system must be mixing, respectively chaotic and ergodic. In order to achieve this goal the Nosé-Hoover scheme can be generalized yielding more nonlinear equations of motion than the original method. However, such "stronger" thermostating forces affecting more profoundly the original dynamics of the subsystem to be thermostated pose the question to which extent the original dynamics of the subsystem still plays a role at all. In any case, our discussion clearly shows that a great variety of deterministic and time-reversible thermal reservoirs exists. This fact one may particularly want to take into account with respect to suspected universalities of NSS as concluded from applications from Gaussian and Nosé-Hoover thermostats only.

V. SUMMARY AND CRITICISM OF GAUSSIAN AND NOSÉ-HOOVER THERMOSTATS

The approach to nonequilibrium transport reviewed in the previous chapters yields NSS on the basis of non-Hamiltonian equations of motion. This dynamics results from employing deterministic and time-reversible thermal reservoirs that control the temperature of a subsystem under nonequilibrium constraints. The Gaussian and the Nosé-Hoover thermostat constructed before serve as two famous examples of such mechanisms. Both reservoirs have been applied to the periodic Lorentz gas driven by an external electric field, and the resulting NSS have been analyzed with respect to their chaos and transport properties. In the following we focus onto what we consider to be generic properties of NSS associated with Gaussian and Nosé-Hoover dynamics. Our summary is accompanied by a critical discussion of these fundamental features as far as a possible universal description of NSS, irrespective of the specific type of thermostat, is concerned. This assessment will set the scene for the subsequent two chapters.

A. Non-Hamiltonian dynamics for nonequilibrium steady states

Constructing NSS requires either to start from a Hamiltonian that models a thermal reservoir of infinitely many degrees of freedom or to use non-Hamiltonian equations of motion, see Section I.B. As an example, in Section II.B we have derived the stochastic Langevin equation from a Hamiltonian defining a thermal reservoir that consists of infinitely many harmonic oscillators. The resulting equation turned out to be dissipative, non-deterministic and non time-reversible thus providing a well-known example of non-Hamiltonian dynamics. This dynamics particularly results from the fact that the equations of motion of the infinitely many reservoir degrees of freedom were eliminated in the course of the derivation, supplemented by some further approximations.

Actually, as we have demonstrated in Section II.C, projecting out spurious reservoir degrees of freedom typically³³ yields a non-uniform probability density for the thermostated subsystem while the combined distribution of subsystem plus thermal reservoir is still uniform, respectively microcanonical. The non-uniformity of the projected equilibrium density may be taken as an indication of some phase space contraction in the associated variables which is not present in the original phase space volume preserving Hamiltonian dynamics of the full system. Indeed, in case of the Langevin equation and for Gaussian and Nosé-Hoover dynamics the equations of motion of the respectively thermostated subsystem are always non-Hamiltonian.

We thus argue that the non-Hamiltonian character results from conveniently simplifying the equations of motion of subsystem plus reservoir by considering the relevant degrees of freedom only while neglecting others. Hence, such a non-Hamiltonian formulation is in principle very well compatible with a Hamiltonian description of the complete combination of subsystem plus reservoir.

Since the use of non-Hamiltonian dynamics for modeling NSS was [Eyi92,Coh92] and is [Lar03] often criticized, we illustrate our arguments by means of a very simple example. Let us consider the two-dimensional baker map acting onto the unit square,

$$B(x, y) = \begin{cases} (2x, (y+1)/2) & , \quad 0 \leq x < \frac{1}{2} \\ (2x-1, y/2) & , \quad \frac{1}{2} \leq x \leq 1 \end{cases} . \quad (58)$$

This map squeezes the unit square along the vertical direction while stretching it horizontally such that the area is preserved. The resulting rectangle is cut in the middle, and both parts are put on top of each other yielding the dynamics depicted in Fig. 12. The corresponding equations of motion read

$$(x_{n+1}, y_{n+1}) = B(x_n, y_n) , \quad (59)$$

where $n \in \mathbb{N}$ holds for the discrete time.

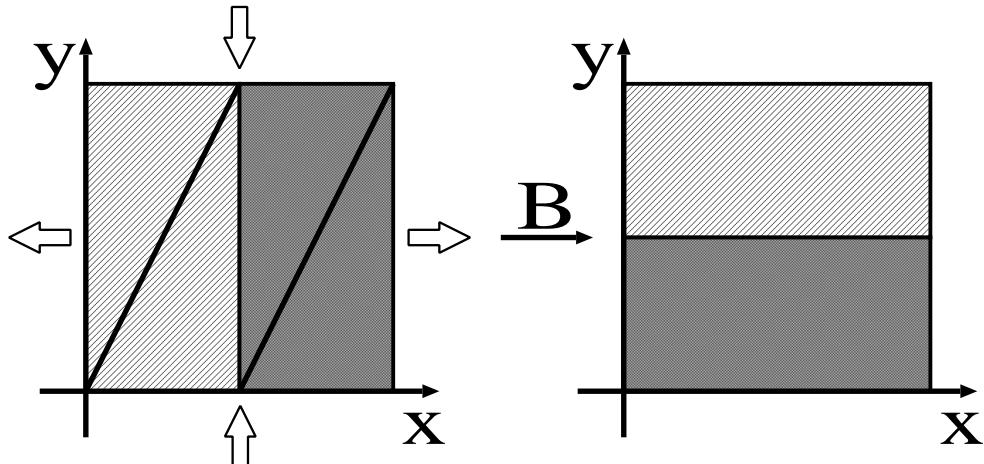


FIG. 12. Sketch of the baker map defined by Eq. (58): a unit square is stretched horizontally and squeezed vertically by preserving its unit area. The resulting rectangle is cut in the middle, and both parts are put on top of each other forming again a unit square. The two diagonal lines in the left part of the figure represent the one-dimensional Bernoulli shift acting onto the x variable only, which determines the dynamics of the baker map along the horizontal axis.

As already remarked in Refs. [Gas98a,Gas03], it appears that the baker map was first defined and studied by Seidel in 1933 [Sei33] who, in turn, gives informal credit to Birkhoff for its invention. Later on this map was considered by Hopf [Hop37]. Eventually, it became very popular starting from the discussion by Arnold and Avez [Arn68], who also coined the name.³⁴ The baker map is one of the most simple chaotic dynamical systems serving as a standard model in many textbooks on nonlinear dynamics, see,

³³A counterexample was provided by subsystem and reservoir living altogether in three dimensions and projecting out two of them, see Fig. 2.

³⁴Both Seidel and Hopf used the baker map as an example for a system that is metrically transitive, or mixing, respectively. Arnold and Avez proved that this map is Bernoulli exhibiting the property of a K-system with positive metric entropy. Seidel originally discussed a baker with stretching/squeezing factors of 10, respectively 1/10.

e.g., Refs. [Sch89,Ott93,Gas98a,Dor99]. Starting from the work by Gaspard [Gas92a] the baker dynamics became extremely popular in form of an analytically tractable model for nonequilibrium transport, the spatially extended so-called multibaker map [Gas93,Tas95,Tel96,Vol97,Gas97,Bre98,Vol98,Gas98c,Gil99a,Gil99b,Tas99,Tas00] [Vol00,Ron00b,Gil00b,Gil00a,Tel00,Gil01,Vol02,Woj02,Gar02,Gil03,Gas03,Woj03,Vol03].³⁵ Even so-called thermostated multibaker maps have been constructed and analyzed from the point of view of mimicking the action of Gaussian and Nosé-Hoover thermostats [Tel96,Vol97,Bre98,Vol98,Gil99a,Gil99b,Vol00,Ron00b,Gil00a,Vol03]. However, in this review we restrict ourselves to the original formulation of Gaussian and Nosé-Hoover dynamics in terms of differential equations only. Corresponding time-discrete dissipative models are reviewed particularly in Refs. [Tel00,Vol02,Dor99].

That the baker map Eq. (58) is area-preserving can be confirmed by computing its Jacobian determinant. The map is furthermore invertible and, even more, shares a specific symmetry property that is usually referred to as *reversibility* in time-discrete maps.³⁶ These properties are analogous to respective features in time-continuous Hamiltonian dynamical systems.³⁷ It is not our purpose to give a detailed account concerning the dynamical systems properties of the baker map.³⁸ We just wish to convey that it is a widely studied standard model mimicking, at least to some extent, a Hamiltonian chaotic dynamical system on the level of time-discrete equations of motion.

In order to illustrate our above discussion about the origin of non-Hamiltonian dynamics we now project out one variable of the baker map. This can be performed starting from the Liouville equation for the baker map³⁹ by simply integrating over the y -variable, see Ref. [Dor99] for the detailed calculation. However, x and y are already nicely decoupled in Eq. (58) with respect to the direction of the projection. One may therefore immediately conclude that the time-discrete Liouville equation determining the evolution of the probability density along the x -axis only must be governed by the action of the one-dimensional map

$$x_{n+1} \equiv B_x(x_n) = 2x_n \mod 1 , \quad (60)$$

This *Bernoulli shift* is included in Fig. 12. Its Jacobian determinant is equal to two, hence this map is uniformly expanding and does not preserve the phase space volume. The baker map thus provides a simple example of a system whose complete two-dimensional dynamics is area-preserving, whereas by projecting out one variable the associated one-dimensional equations of motion are dissipative.

Curiously, the equilibrium density of the Bernoulli shift is still uniform, as for the original baker map, whereas in Section II.C the probability densities obtained from projecting out reservoir degrees of freedom were typically non-uniform. In order to more closely connect to these results one may simply rotate the unit square of the baker map by 45 degrees [Hoo98b]. Now the density projected upon the horizontal line by integrating over the vertical axis will be non-uniform, whereas the full baker map is still area-preserving. Unfortunately, in contrast to the non-rotated case here the dynamics along the horizontal, respectively the vertical axes are not decoupled anymore,⁴⁰ and it is not straightforward to extract equations of motion governing the dynamics along the x -axis only.

This simple example demonstrates again that non-Hamiltonian dynamics may fit very well together with Hamiltonian equations of motion for the complete system consisting of subsystem plus thermal reservoir. In such a case a non-Hamiltonian dynamics just results from conveniently projecting out superfluous (reservoir) degrees of freedom such as the passive y -variable in the baker map, see also Rondoni et al. [Ron02a,Eva02a] for an analogous argumentation.

³⁵For multibaker maps the unit cell of the baker map is periodically continued along the x -axis. The single cells are then coupled with each other by mapping, say, the left vertical strip of the left part in Fig. 12 into the next cell to the right while mapping the right vertical strip into the next cell to the left, and so on.

³⁶A map B is called *reversible* if there exists an involution G , $GG = 1$, in phase space reversing the direction of time, $BGB = G$ [Rob92]. Thus reversibility in maps is more than the existence of an inverse. However, note that such a reversibility does not necessarily imply time-reversibility [Dol00] and that there is a controversy of how to define time-reversibility in maps [Rob92,Tas95,Hoo96b,Hoo98b,Bre98,Gil99b,Gas98a,Vol02].

³⁷However, note that the baker map does not share the property of being symplectic, in contrast, for example, to the standard map [Ott93,Mei92].

³⁸Let us mention only some very basic characteristics: Apart from being mixing and a K-system implying chaotic behavior the baker map is also hyperbolic [Dor99]. Strictly speaking it is not Anosov because it is not differentiable at the point of discontinuity [Gas98a].

³⁹The time-discrete Liouville equation is usually called *Frobenius-Perron equation* in dynamical systems theory [Dor99, Gas98a, Ott93].

⁴⁰This is related to the fact that we are not projecting onto the unstable manifold only, which is usually the adequate choice for performing a projection.

In our view a non-Hamiltonian description thus emerges very naturally in equations designed to model NSS, and in this respect Gaussian and Nosé-Hoover thermostats are not particularly artificial or unusual.

On the other hand, one should keep in mind that Gaussian and Nosé-Hoover reservoirs have not been derived starting from a purely Hamiltonian dynamics, see, e.g., again the derivation of the Langevin equation in Section II.B for comparison. Moreover, in contrast to the projected baker dynamics and to the Langevin equation the former two types of dynamics are even time-reversible. Of course, for Gauss and Nosé-Hoover there exists the generalized Hamiltonian approach discussed in Section IV.C.2, however, it only represents a formal analogy and not a rigorous Hamiltonian derivation. We therefore emphasize again that Gaussian and Nosé-Hoover dynamics yield only a *heuristic modeling* of NSS rather than providing a theory starting from first principles. Hence, one cannot rule out in advance that the properties of dynamical systems thermostated that way may depend on specificities of these thermal reservoirs. This should be taken into account when searching for universal properties of NSS along the lines of this approach.

B. Phase space contraction and entropy production

The periodic Lorentz gas driven by an external electric field yielded NSS after connecting this model to either the Gaussian or to the Nosé-Hoover thermostat. Both types of thermostated systems were characterized by an identity between the absolute value of the average rate of phase space contraction and the thermodynamic entropy production in terms of Joule's heat, see Sections III.B.1 and IV.C.1. This identity represents a basic property of ordinary Gaussian and Nosé-Hoover dynamics and furnishes a crucial link between dynamical systems quantities and transport properties. Interestingly, even the stochastic Langevin equation Eq. (1) supplemented by an external electric field exhibits this identity, as one can easily verify. However, in contrast to Gaussian and to Nosé-Hoover dynamics this equation is less amenable to an analysis in terms of dynamical systems theory because of the stochastic forces involved. We now show that this identity is in fact linked to a more general relationship between phase space contraction and entropy production, which holds irrespective of the specific type of dynamical system considered. In our presentation we follow Ref. [And85], for other derivations see particularly Refs. [Eva85a,Eva90b,Gas97,Dor99,Gal99,Rue99b,Det00a,Eva02a].

Let us start from the general dynamical system

$$\dot{\mathbf{x}} = \mathbf{F}(\mathbf{x}) , \quad (61)$$

where \mathbf{x} and \mathbf{F} denote vectors in a k -dimensional phase space $\Gamma \subset \mathbb{R}^k$, $k \in \mathbb{N}$. For convenience here we shall not distinguish between position and velocity components. One may now inquire about the average rate of entropy production in this system by using *Gibbs definition of entropy* [Pen79,Eva90b,Rue99b,Gas98a,Det00a]

$$S_G := - \int_{\Gamma} d\Gamma \rho \ln \rho . \quad (62)$$

Here $\rho \equiv \rho(x_1, x_2, \dots, x_k)$ denotes the distribution function of the *complete* dynamical system Eq. (61) determined by the Liouville equation Eq. (36) and $d\Gamma := dx_1 dx_2 \dots dx_k$ represents a volume element of the phase space Γ . In order to calculate the Gibbs entropy production we differentiate Eq. (62) by employing the Leibnitz rule, which yields

$$\frac{dS_G}{dt} = - \int_{\Gamma} d\Gamma (1 + \ln \rho) \frac{\partial \rho}{\partial t} - \sum_i \int_{\Gamma'} d\Gamma' \rho \ln \rho F_i|_{\partial \Gamma_i} \quad (63)$$

with $d\Gamma' := dx_1 \dots dx_{i-1} dx_{i+1} \dots dx_k$ and F_i defined at the boundary $\partial \Gamma_i$. The derivative $\partial \rho / \partial t$ can be substituted by using the Liouville equation Eq. (36) leading to

$$\frac{dS_G}{dt} = \int_{\Gamma} d\Gamma \rho \nabla \cdot \mathbf{F} + \int_{\Gamma} d\Gamma \rho \ln \rho \nabla \cdot \mathbf{F} + \int_{\Gamma} d\Gamma (1 + \ln \rho) \mathbf{F} \cdot \nabla \rho - \sum_i \int_{\Gamma'} d\Gamma' \rho \ln \rho F_i|_{\partial \Gamma_i} . \quad (64)$$

Performing integration by parts the second term on the right hand side of the above equation precisely cancels with the last two terms in the same equation. The final result thus reads

$$\frac{dS_G}{dt} = \int_{\Gamma} d\Gamma \rho \nabla \cdot \mathbf{F} , \quad (65)$$

which means that the rate of Gibbs entropy production is always identical to the average rate of phase space contraction defined by Eq. (27). This important identity was noted by Gerlich [Ger73] and was subsequently discussed in various settings by other authors [Dob76a,Dob76b,Ste79,And82]. A very lucid and clear statement of this

identity is due to Andrey [And85]. In the context of Gaussian and Nosé-Hoover dynamics the importance of the relationship Eq. (65) was particularly emphasized in Refs. [Eva85a,Bre96,Hol87,Hoo87,Pos88,Rue96,Rue97a,Gal99] [Rue99b,Hoo99,Dor99,Rue03].

As we have mentioned at the beginning of Chapter I, it appears that there is no generally accepted definition of a thermodynamic entropy in nonequilibrium situations. Some authors considered the Gibbs entropy Eq. (62) to be a suitable candidate for such a nonequilibrium entropy [Eva90b, Gal99, Rue99b, Hoo99]. However, in our view using this concept causes a number of problems.

First of all, Eq. (65) tells us that for phase space volume preserving dynamics the Gibbs entropy production is strictly zero. This fact is problematic [Nic98, Det00a], for example, in case of diffusion in Hamiltonian dynamical systems under concentration gradients imposed by flux boundary conditions [Gas97, Gas98a], see also Ref. [Eck99a] for a Hamiltonian modeling of a heat flow under temperature gradients. In both nonequilibrium situations there is a well-defined irreversible entropy production while the Gibbs entropy production is strictly zero, since there is no non-Hamiltonian thermostating.

Secondly, dissipative dynamical systems usually exhibit a *negative* average rate of phase space contraction. Specific examples are provided by the Gaussian and the Nosé-Hoover thermostated driven Lorentz gas, see Eqs. (28) and (48). According to Eq. (65) the Gibbs entropy production is also negative reflecting a contraction of the system onto a subset in phase space such as a fractal attractor. The decrease of the Gibbs entropy thus measures the fact that the dynamical system is getting “more ordered” in phase space. However, a negative thermodynamic entropy production in NSS appears to be in contradiction with the second law of thermodynamics.

In our earlier derivations of Sections III.B.1 and IV.C.1, which specifically concerned the Gaußsian and the Nosé-Hoover thermostated Lorentz gas, we circumvented this sign problem, since we did not start from the Gibbs entropy production. Instead, we directly computed the average rates of phase space contraction by realizing afterwards that the *absolute* values yielded the thermodynamic entropy production in form of Joule’s heat. This enabled us to “invert the sign” and to establish the identity without entering into the discussion concerning a negative Gibbs entropy production.

A more physical interpretation of the sign reversal may be obtained as follows [Che93a, Rue96, Dor99, Hoo99]: Let us consider a balance equation for the total entropy production of a subsystem under nonequilibrium conditions, in analogy to Eq. (35). The source term stands for the entropy production within the subsystem, whereas the flow term holds for the average heat transfer from the subsystem to the thermal reservoir. The reservoir fully absorbs the entropy produced by the subsystem such that in a NSS the average entropy production of subsystem plus thermal reservoir is zero. Hence, from the side of the thermal reservoir the entropy flux must be *positive* causing a positive entropy production in the reservoir. This entropy production may be identified as the relevant one in the sense of irreversible thermodynamics thus yielding the sign reversal. However, in detail this explanation is debatable [Nic96, Gas97, Gas98a, Nic98, Gil99a, Dae99], because we did not identify a positive entropy production *within* the subsystem itself.

More refined approaches resolve the sign problem by using methods of coarse graining for the phase space densities as they enter into the definition of the Gibbs entropy Eq. (62) [Bre96, Nic96, Vol97, Gas97, Vol98, Bre98, Nic98] [Gil99a, Tas99, Dae99, Gas98a, Gil00b, Gil00a, Tas00, Tel00, Dor02, Vol02, Mae03a, Vol03]. Such a coarse grained formulation may be motivated by a second basic deficiency of the Gibbs entropy [Nic96, Gas97, Dae99, Gil99a, Gas98a]: As we have shown in Sections III.B.3 and IV.C.3, in deterministically thermostated systems the phase space density typically contracts onto fractal attractors. However, the fractal structure implies that the probability densities characterizing the associated NSS must be singular and non-differentiable. Consequently, they are no well-defined mathematical objects anymore.⁴¹ Correspondingly, the integration in Eq. (62) is also not well-defined anymore.⁴² As a consequence of the formation of these fractal structures it was thus proposed by many authors to use *coarse-grained* Gibbs entropies in order to arrive at a suitable concept of a nonequilibrium entropy, see the long list of references cited above. Up to now these methods have mostly been worked out for time-discrete dynamical systems such as multibaker-maps for which different types of coarse graining have been explored. Concerning further details we may refer, e.g., to Refs. [Gil99a, Gas98a, Tel00, Vol02] providing recent summaries of this issue.

In the light of this criticism it may appear rather surprising that for the Gaussian and for the Nosé-Hoover thermostated driven Lorentz gas the ordinary Gibbs entropy production can nevertheless be fully identified with the thermodynamic entropy production in terms of Joule’s heat subject to a sign reversal. A related fact that further contributes to this

⁴¹In contrast, the corresponding probability *measures* may still be well-defined. Typically, these are SRB measures being smooth along unstable but fractal along stable manifolds [Gas98a, Dor99, Gal99, Rue99b, You02, Gal03].

⁴²In this case the integral should be replaced by a Lebesgue-Stieltjes integral over the invariant measure [Dor99, Gas98a].

surprise is that Gibbs' formulation assesses the entropy of a system with respect to *all* phase space variables and with respect to their *complete* deterministic dynamics in time. This is at variance to concepts like coarse-grained Gibbs entropies or Boltzmann entropies. Here there is already a loss of information, because these quantities are not employing the complete phase space densities or respective probability measures as determined by the Liouville equation. In a similar vein, a heat flux from a subsystem to a thermal reservoir will usually involve only a specific fraction of all phase space variables. From the point of view of Clausius definition of entropy production, see Section III.B.1, the Gibbs entropy may thus measure spurious contributions in comparison to a thermodynamic entropy production by assessing phase space coordinates that are not involved in any heat transfer to a thermal reservoir.

All these physical arguments support again the use of a respectively coarse grained entropy that only assesses the physically relevant contributions to a thermodynamic entropy production. We believe that such a formulation of a nonequilibrium entropy should be compatible with the one of Clausius in terms of a heat transfer. From that point of view there is no reason why phase space contraction, or the respective Gibbs entropy production, should always be identical to the thermodynamic one. One may suspect that such an identity may rather be characteristic of the specific family of thermostats investigated so far.

This hypothesis will be verified by presentings generic families of counterexamples where the identity between phase space contraction and thermodynamic entropy production, respectively between Gibbs and thermodynamic entropy production, is not fulfilled. In order to qualify as counterexamples alternative models of thermal reservoirs must share some basic physical properties with Gaussian and Nosé-Hoover thermostats, such as being dissipative, deterministic and time-reversible. Furthermore, there should be an adequate physical interpretation of the thermostating mechanism. Such counterexamples will be introduced and analyzed in the following two chapters.

C. Transport coefficients and dynamical systems quantities

If there exists an identity between the average phase space contraction rate and thermodynamic entropy production, it is straightforward to link transport coefficients with dynamical systems quantities. Interestingly, for the field-dependent conductivity $\sigma(\varepsilon)$ of both the Gaussian and the Nosé-Hoover thermostated driven periodic Lorentz gas one obtains the same functional relationship reading

$$\sigma(\varepsilon) = -\frac{T}{\varepsilon^2} \sum_{i=1}^N \lambda_i(\varepsilon) \quad , \quad (66)$$

cp. to Eqs. (33) and (51), where N denotes the total number of field-dependent Lyapunov exponents $\lambda_i(\varepsilon)$ and T stands for the temperature. The existence of such a simple functional relationship between chaos quantities and transport coefficients is typical for Gaussian and Nosé-Hoover thermostated dynamical systems, see Sections III.B.2 and IV.C.1 for further details.

Surprisingly, by using the escape rate approach to chaotic transport outlined in Section I.A, independently very similar formulas were derived for the very different class of *open Hamiltonian* dynamical systems, where there is an escape of phase space points due to absorbing boundaries. This second fundamental approach to NSS does not require any modeling of thermal reservoirs, hence by default it does not involve any phase space contraction. We will now provide a brief summary concerning formulas linking transport coefficients to dynamical systems quantities as they emerge from both the escape rate and the thermostated systems approach. The resulting different but related formulas will be compared in detail and possible crosslinks between them will be critically assessed.

For sake of simplicity we mainly restrict ourselves again to the periodic Lorentz gas. We start with the driven Lorentz gas under application of a Gaussian thermostat for which $N = 2$ in Eq. (66). In order to connect to the escape rate approach we reformulate this equation as follows [Gas98a,Gil01,Rue96]: For the Gaussian thermostated Lorentz gas the sum of Lyapunov exponents on the right hand side consists only of a positive one, $\lambda_+(\varepsilon)$, and a negative one, $\lambda_-(\varepsilon)$, see Eq. (33). Both Lyapunov exponents are defined with respect to the invariant measure of the dynamical system which is concentrated on the field-dependent fractal attractor \mathcal{A}_ε . We now indicate this dependence explicitly by writing $\lambda_\pm(\varepsilon) \equiv \lambda_\pm(\mathcal{A}_\varepsilon)$.

As was proven in Refs. [Che93a,Che93b], under certain conditions there holds the *Pesin identity* [Eck85,Ott93,Bec93,Gas98a,Dor99] between the Kolmogorov-Sinai entropy $h_{KS}(\mathcal{A}_\varepsilon)$ and the positive Lyapunov exponent on the attractor, $h_{KS}(\mathcal{A}_\varepsilon) = \lambda_+(\mathcal{A}_\varepsilon)$, for the Gaussian thermostated driven Lorentz gas. Having this in mind we rewrite the right hand side of Eq. (66) as

$$-\sum_{i=1}^2 \lambda_i(\mathcal{A}_\varepsilon) = -\lambda_+(\mathcal{A}_\varepsilon) - \lambda_-(\mathcal{A}_\varepsilon)$$

$$\begin{aligned}
&= -h_{KS}(\mathcal{A}_\varepsilon) - \lambda_-(\mathcal{A}_\varepsilon) \\
&= |\lambda_-(\mathcal{A}_\varepsilon)| - h_{KS}(\mathcal{A}_\varepsilon)
\end{aligned} \tag{67}$$

The domain of the escape rate approach is particularly the description of diffusion processes, see Section I.A. Accordingly, since the Einstein relation Eq. (34) holds for the Gaussian thermostated driven Lorentz gas [Che93a,Che93b] the electrical conductivity $\sigma(\varepsilon)$ on the left hand side of Eq. (66) may be replaced by the diffusion coefficient D , $D = T\sigma(\varepsilon)$ ($\varepsilon \rightarrow 0$). This yields as a final result [Gas98a,Gil01,Rue96,Bre96]

$$D = \lim_{\varepsilon \rightarrow 0} \left(\frac{T}{\varepsilon} \right)^2 (|\lambda_-(\mathcal{A}_\varepsilon)| - h_{KS}(\mathcal{A}_\varepsilon)) . \tag{68}$$

A corresponding formula from the escape rate approach to chaotic diffusion is obtained as follows [Gas90,Gas92b,Gas93,Gas95a,Dor95,Gas95b,Kla96,Kla99a,Gas98a,Dor99]: We consider a slab of the periodic Lorentz gas with reflecting or periodic boundaries, say, in the vertical direction while in the horizontal direction we use absorbing boundaries a distance L apart from each other. We do not apply any external field but just look at the diffusion of an initial ensemble of point particles along the x -axis. Choosing the density of scatterers such that the periodic Lorentz gas is normal diffusive, see Section II.D, we expect an exponential decrease of the number N of particles in time t according to

$$N(t) = N(0) \exp(-\gamma_{esc} t) , \tag{69}$$

where $N(0)$ stands for the initial number of particles at time zero. Solving the one-dimensional diffusion equation with absorbing boundary conditions yields

$$D = \lim_{L \rightarrow \infty} \left(\frac{L}{\pi} \right)^2 \gamma_{esc} , \tag{70}$$

that is, the diffusion coefficient is obtained in terms of the *escape rate* which strictly speaking depends on L , $\gamma_{esc} \equiv \gamma_{esc}(L)$. Let us now assume that the *Pesin identity for open systems* holds for the open periodic Lorentz gas,⁴³

$$\gamma_{esc} = \lambda_+(\mathcal{R}_L) - h_{KS}(\mathcal{R}_L) . \tag{71}$$

Here $\gamma_{esc} \equiv \gamma_{esc}(\mathcal{R}_L)$ denotes the *escape rate* of particles with respect to the fractal repeller \mathcal{R}_L . Combining this equation with Eq. (70) leads to the fundamental result

$$D = \lim_{L \rightarrow \infty} \left(\frac{L}{\pi} \right)^2 (\lambda_+(\mathcal{R}_L) - h_{KS}(\mathcal{R}_L)) . \tag{72}$$

Obviously, the functional forms of Eqs. (68) and (72) are just the same. However, we emphasize again that both the types of dynamical systems considered and the approaches by which these equations have been derived are very different.

On the other hand, for both derivations the key was to identify a quantity providing a link between chaos and transport properties. For thermostated systems this role is played by the average phase space contraction rate κ defined in Eq. (27). In case of open Hamiltonian systems the escape rate γ_{esc} serves for the same purpose. This analogy was first seen by Breymann, Tél and Vollmer [Bre96] and by Ruelle [Rue96]. These authors suggested to define a Gibbs entropy for open dynamical systems, in parallel to the Gibbs entropy of closed but thermostated, phase space contracting dynamical systems, related to the concept of conditionally invariant measures. Here the probability measures of particles remaining in the system, respectively the corresponding probability densities, are renormalized in time in order to make up for the loss of absorbed particles. Along these lines the Gibbs entropy production for open systems can be identified with the escape rate, $dS_G/dt = \gamma_{esc}$. On the other hand, for closed systems we have shown in the previous section that the Gibbs entropy production is equal to the average rate of phase space contraction, see Eq. (65). Hence, if the rates of Gibbs entropy production for closed and open systems were the same both Eqs. (68) and (72), that apply to very different dynamical systems, yielded the same transport coefficients in

⁴³So far this identity is only proven for Anosov diffeomorphisms, see, e.g., Refs. [Eck85,Bec93,Dor99,Gas98a] for outlines concerning this generalization of Pesin's identity and further references therein.

terms of dynamical systems quantities. This was indeed shown to be the case for some simple model systems, that is, (multi)baker maps, under periodic, absorbing and flux boundary conditions thus suggesting an equivalence of these very different nonequilibrium ensembles [Mor96b,Vol97,Vol98,Gil99a,Gil99b,Gil00a,Tel00,Vol02,Vol03]. Tél et al. have furthermore considered the situation of a hybrid system that is both open and dissipative [Tel96,Tel00,Vol02]. By solving the corresponding Fokker-Planck equation with absorbing boundaries and employing again the Pesin identity for open systems they arrived at the generalized formula (see also Ref. [Gas98a])

$$D \left(\frac{\pi}{L} \right)^2 + \frac{\sigma^2 \varepsilon^2}{4D} = \sum_{\lambda_i > 0} \lambda_i (\mathcal{R}_L) - h_{KS}(\mathcal{R}_L) \quad (L \rightarrow \infty, \varepsilon \rightarrow 0) \quad . \quad (73)$$

Carrying out the limit of $\varepsilon \rightarrow 0$ eliminates the second term on the left hand side yielding precisely Eq. (72) of the escape rate approach if applied to the Lorentz gas. On the other hand, performing $L \rightarrow \infty$ eliminates the first term on the left hand side. The conductivity may then be replaced again by Einstein's formula Eq. (34). Taking into account that for the Gaussian thermostat the temperature T should be replaced by $T \equiv T/2$, see Section III.B.1, and assuming that in the limit of $\varepsilon \rightarrow 0$ the spectrum of Lyapunov exponents exhibits conjugate pairing, $\sum_{\lambda_i > 0} \lambda_i = \sum_{\lambda_i < 0} |\lambda_i|$, one recovers the result for the thermostated Lorentz gas Eq. (68).

We finally outline a third basic approach linking transport coefficients to dynamical systems quantities as recently formulated by Gilbert et al. [Gil01, Gas01, Cla02]. Here particularly diffusion in closed volume-preserving dynamical systems has been considered. Starting from the diffusion equation with periodic boundary conditions the solution for the diffusion coefficient reads

$$D = \lim_{L \rightarrow \infty} \left(\frac{L}{2\pi} \right)^2 \gamma_{dec} \quad . \quad (74)$$

This result is in formal analogy to Eq. (70), however, here γ_{dec} denotes the *decay rate* by which an equilibrium state is approached. By solving the Liouville equation of the respective dynamical system γ_{dec} can be related to the second largest eigenvalue of the Liouville operator associated with the corresponding hydrodynamic mode of diffusion of the dynamical system, see, e.g., Refs. [Kla96, Kla99a]. The crucial observation is now that this eigenvalue is linked to the Hausdorff dimension of the respective mode. Thus, the diffusion coefficient in Eq. (74) can be written as a function of the fractal dimension of the second largest eigenmode of the Liouville equation [Gil01, Gas01]. For systems with two degrees of freedom which are periodically continued in one direction over a length L one gets

$$D = \lim_{L \rightarrow \infty} \left(\frac{L}{2\pi} \right)^2 \lambda_+ (d_H(2\pi/L) - 1) \quad , \quad (75)$$

where the Hausdorff dimension d_H is a function of the length of the system, or respectively of the wavenumber $k = 2\pi/L$ of the corresponding hydrodynamic mode. λ_+ denotes again the positive Lyapunov exponent of the system. This approach has been worked out in detail for a multibaker map [Gil01] as well as for diffusive and reactive-diffusive billiards of Lorentz gas type [Gas01, Cla02].

In order to compare Eq. (75) with the previous two formulas Eqs. (68) and (72) one may employ the Kaplan-Yorke formula, respectively Young's formula, which in case of the two-dimensional periodic Lorentz gas with a constrained kinetic energy reads [Eck85, Ott93, Gil01, Che93a]⁴⁴

$$d_I = 2 + h_{KS}/|\lambda_-| \quad . \quad (76)$$

This formula links the information dimension d_I of a fractal set to the Kolmogorov-Sinai entropy h_{KS} and to the negative Lyapunov exponent λ_- of the corresponding dynamical system. By using this equation Eq. (68) can be rewritten as

$$D = \lim_{\varepsilon \rightarrow 0} \left(\frac{T}{\varepsilon} \right)^2 \lambda_+(\mathcal{A}_\varepsilon) (3 - d_I(\mathcal{A}_\varepsilon)) \quad . \quad (77)$$

It appears that this formula was first derived in Ref. [Eva00]. Analogously, Eq. (72) reads

⁴⁴We remark that so far this formula has only been proven for two-dimensional Anosov diffeomorphisms with an ergodic measure on compact manifolds, see Refs. [Eck85, Ott93] for further literature.

$$D = \lim_{L \rightarrow \infty} \left(\frac{L}{\pi} \right)^2 \lambda_+(\mathcal{R}_L) (3 - d_I(\mathcal{R}_L)) . \quad (78)$$

In both cases the information dimension d_I is furthermore identical to the Hausdorff dimension d_H of the respective fractal set and may be replaced respectively [Che93a,Che93b,Gas95a].

In conclusion, all three equations Eqs. (75), (77) and (78) relate the diffusion coefficient to the largest positive Lyapunov exponent of the corresponding dynamical system times a term containing the information dimension of the associated fractal structure, which in Eq. (75) is a fractal hydrodynamic mode, in Eq. (77) a fractal attractor and in Eq. (78) a fractal repeller.⁴⁵ Hence, on this level there is quite a formal analogy even between all three approaches. One may thus indeed wonder whether these formulas form a kind of general backbone of nonequilibrium transport in terms of dynamical systems theory [Bre96,Tel96,Rue96]. We remark that, in addition, there exist very interesting, simple formulas by which transport coefficients can be calculated in terms of periodic orbits, see, e.g., Ref. [Van92] for the electrical conductivity and Refs. [Cvi95,Cvi92,Gas98a,Cvi03] for the diffusion coefficient. However, these formulas are conceptually rather different from the ones discussed above. Therefore we do not discuss them here by instead referring to the respective literature, see, e.g., Ref. [Cvi03] for an overview.

Despite their striking formal analogy one may not overlook that all three equations concern very different physical settings [Coh92,Det00a,Gil01]: Eq. (78) applies to diffusion in open Hamiltonian dynamical systems without external fields, where the link between chaos and transport is formed by the rate assessing the escape from the fractal repeller. Eq. (75) concerns diffusion in closed Hamiltonian dynamical systems, again without using external fields, however, here there is no repeller. Instead, the fractality of the hydrodynamic mode of diffusion is assessed. In contrast to these two relations, Eq. (77) originally started from the current generated in a non-Hamiltonian dynamical system under application of external fields in combination with a specific thermostat. Here the link between chaos and transport is provided by the average phase space contraction rate onto the fractal attractor. Particularly in case of Eqs. (77) and (78) the physical situations involved remain inherently different.

That both equations can nevertheless be derived from a ‘master formula’ is nicely demonstrated by the hybrid equation Eq. (73). However, the left hand side of this equation represents obviously just the sum of the left hand sides of Eqs. (68) and (72) supplemented by the prefactors from the respective right hand sides. If we add the prefactor-free right hand sides of these two equations as well we obtain, by using the original formulation in the first line of Eq. (67) instead of the right hand side of Eq. (68), $-\lambda_+(\mathcal{A}_\varepsilon) - \lambda_-(\mathcal{A}_\varepsilon) + \lambda_+(\mathcal{R}_L) - h_{KS}(\mathcal{R}_L)$ ($L \rightarrow \infty, \varepsilon \rightarrow \infty$). By assuming that, in the above limits, $\lambda_\pm(\mathcal{A}_\varepsilon) = \lambda_\pm(\mathcal{R}_L)$ and that, as before, conjugate pairing holds, $\lambda_+ = -\lambda_-$, we recover the right hand side of Eq. (73) for the periodic Lorentz gas. Hence, one may argue that Eq. (73) represents an additive combination of both formulas. That a more intricate, common root of these two formulas going beyond this equation exists, possibly even combining these two relations with the third one in terms of hydrodynamic modes, appears to be very unlikely to us.

We may furthermore emphasize again that the validity of Eq. (68) stands and falls with the existence of the identity between phase space contraction and thermodynamic entropy production. In the previous section we have already casted doubt on the general validity of this identity for dissipative systems. Indeed, the two key quantities linking thermodynamics to chaotic dynamics discussed above measure quite different physical processes: The escape rate merely assesses the absorption of the number of phase space points, or particles, at some boundary, whereas the phase space contraction rate is defined with respect to the full details of the dynamical system in all variables. As we have outlined to the end of the previous section it is thus conceivable that the phase space contraction rate contains spurious information as far as thermodynamic entropy production and transport processes are concerned. We are not aware that yet there are any counterexamples questioning the validity of the formulas emerging from the escape rate and the closed Hamiltonian systems approach. However, as we will argue in the remaining chapters, for the thermostated systems approach the situation appears to be much more delicate.

Concerning practical applications for the calculation of transport coefficients it seems that these three formulas do not provide more efficient computational schemes than, say, Einstein formulas or Green-Kubo relations. As far as we can tell, in most cases dynamical systems quantities such as Lyapunov exponents and Kolmogorov-Sinai entropies are more difficult to compute than statistical averages defined within the framework of common nonequilibrium statistical mechanics only. With respect to a simplification of the Lyapunov sum rule Eq. (66) for higher-dimensional dynamical systems we may recall that the conjugate pairing rule of Lyapunov exponents is not universal for NSS in dissipative dynamical systems. Boundary thermostats and systems under electric and magnetic fields provide counterexamples, see Section III.B.2 for more details.

⁴⁵In order to make this analogy even closer one may further introduce partial codimensions for the fractal structures in Eqs. (77) and (78), however, this does not appear to be possible for the hydrodynamic mode in Eq. (75) [Gil01].

Irrespective of these rather practical concerns, we may emphasize that the existence of these three formulas linking transport coefficients to dynamical systems quantities provides highly interesting results from a fundamental physical and dynamical systems point of view, and the formal similarity of these different equations remains very remarkable.

D. Fractal attractors characterizing nonequilibrium steady states

Another crucial property of Gaussian and Nosé-Hoover thermostated systems is the existence of fractal attractors underlying NSS. These objects form a fundamental link between the microscopic non-Hamiltonian equations of motion that are, for this type of systems, still deterministic and time-reversible while irreversible transport is exhibited on macroscopic scales. Quantitatively, the existence of these attractors manifests itself in the average phase space contraction rate serving as a link between chaos and transport in dissipative systems, see our discussion in the previous sections.

In Sections III.B and IV.C we have studied the Gaussian and the Nosé-Hoover thermostated driven periodic Lorentz gas as paradigmatic examples for this class of thermostated systems. For the Gaussian type numerical and analytical results provided evidence that in the full accessible phase space the Hausdorff dimension of the attractor is non-integer. In Poincaré surfaces of section, or in respective projections of the phase space, the attractor turned out to be even multifractal; see Figs. 5 and 9 for plots depicting the associated fractal folding. Supported by results for many other Gaussian and Nosé-Hoover thermostated systems it was thus conjectured that the existence of fractal attractors, and of the associated singular probability measures, is generic for non-Hamiltonian dynamical systems in NSS subject to deterministic and time-reversible thermal reservoirs.

How the topology of these attractors changes under variation of the electric field strength was assessed by means of bifurcation diagrams, as discussed in the same sections. For this purpose the positions of the colliding particles at the Lorentz gas disk were plotted as functions of the electric field strength, see Figs. 6 and 10. For both the Gaussian and the Nosé-Hoover thermostated driven periodic Lorentz gas these diagrams revealed intricate bifurcation scenarios. On the other hand, the specific form of these scenarios depends intimately on the type of thermal reservoir used and is already very different for Gaussian and Nosé-Hoover dynamics. Even more, in case of Nosé-Hoover thermostating different bifurcation diagrams were obtained for different values of the coupling strength between subsystem and thermal reservoir. Hence, there is no universality concerning the specific change of the topology of these attractors under variation of the field strength. Whether the mere existence of bifurcations, at least, is typical for the thermostated driven periodic Lorentz gas will be clarified in the following two chapters.

However, instead of applying Gaussian and Nosé-Hoover schemes, thermal reservoirs can be mimicked by introducing *stochastic interactions* between subsystem and reservoir particles. Here we briefly sketch various existing numerical and analytical methods of how to model this second fundamental class of thermostats. We then connect to our discussion concerning the possible universality of fractal attractors in NSS.

One way to introduce a stochastic reservoir is by using a Langevin equation, as was discussed in detail in Section II.B. For molecular dynamics computer simulations this approach was first implemented by Schneider and Stoll [Sch78], see also later work in Ref. [Nos91,Pos00b]. Andersen [And80] proposed a variant of this stochastic bulk thermostat by considering an interacting many-particle system, where at certain time intervals the velocity of a randomly selected particle is chosen randomly from a canonical velocity distribution [All87,Jel88a].

Alternatively, a stochastic sampling of velocities from canonical velocity distributions can be performed at the boundaries of a subsystem. Such *stochastic boundary conditions* were proposed by Lebowitz and Spohn in order to mathematically analyze a three-dimensional random Lorentz gas under a temperature gradient [Leb78]. For molecular dynamics computer simulations this thermostating scheme was implemented by Ciccotti and Tenenbaum [Cic80], again in order to model thermal gradients, see also Refs. [Ten82,Che95,Che97,Pos98,Wag99] for later use of this method in the context of computer simulations. Stochastic boundary conditions will be introduced in full detail later on in Section VII.A. However, for the following discussion it is not necessary to know about such technical details.

A particularly important result for the class of stochastic boundary thermostated models was reported by Goldstein, Kipnis and Ianiro [Gol85]. They studied a system of Newtonian particles maintaining a heat flux due to a temperature field that is modeled by stochastic boundaries and varies with the position at the boundary. A mathematical analysis of this system yielded that there exists a unique invariant probability measure that is absolutely continuous [Eck85,Dor99] with respect to the Lebesgue measure. In other words, in this case the measure is not singular and hence not fractal. This result was claimed to be generic for stochastically thermostated systems [Eyi92,Coh92] thus contradicting the universality of fractal attractors as conjectured from studying Gaussian and Nosé-Hoover thermostated systems [Hol87,Hoo99].

The claim that the physically relevant probability measures are generally smooth in stochastically thermostated systems has been doubted by Hoover et al. on the basis of numerical explorations: In Ref. [Hoo98c] these authors

studied a driven periodic Lorentz gas thermalized by a ‘hybrid’ thermostat consisting of deterministic and stochastic boundaries. Computations of the information dimension of the fractal attractor by evaluating phase space projections such as Fig. 9 indicated a slight deviation from an integer value. Furthermore, they considered a one-dimensional Hamiltonian model for heat conduction (the *ding-a-ling* model) with reservoirs defined by stochastic boundaries [Pos98]. They also investigated an interacting many-particle system under an external field [Pos00b] (the *color conductivity model* [Eva90b]). In the latter two cases they computed the information dimension according to the Kaplan-Yorke conjecture, respectively Young’s formula, cp. to Eq. (76) of the previous section. The numerical results yielded again deviations from integer values. However, this dimension formula relies on the computation of Lyapunov exponents that in turn necessitate to define a Jacobian quantifying the interaction of the subsystem with the stochastic boundaries. To us it appears that the definition which these authors used for the Jacobian is generally ill-defined, hence we cannot consider the numerical results of Refs. [Pos98,Pos00b] to be conclusive.⁴⁶ Thus, whether attractors in stochastically thermostated systems are generally smooth or fractal, and to which extent this property depends on the specific type of subsystem considered, still remains a very open question to us.

Apart from these considerations we may emphasize again that both types of thermal reservoirs define very different classes of dynamical systems: Gaussian and Nosé-Hoover thermostats keep the dynamics deterministic and time-reversible, whereas stochastically thermostated systems render the equations of motion non-deterministic and non-time reversible. The controversy [Gol85,Eyi92,Coh92,Hoo98c,Pos98,Pos00b,Gal03] concerning the type of invariant measure that emerges under application of these two very different types of thermal reservoirs thus boils down to the question which type of thermostat one considers to be more ‘physical’. We furthermore remark that, connected to our discussion in Section V.A, Nicolis and Daems [Nic96,Nic98,Dae99] and Ruelle [Rue97b] argued for the positivity of the thermodynamic entropy production in stochastically thermostated systems.

E. Nonlinear response in the thermostated driven periodic Lorentz gas

According to the numerical results for the thermostated driven periodic Lorentz gas the topology of the attractors does not only depend on the specific type of thermal reservoir that has been applied, but it is also very sensitive to variations of the external field. From that point of view it is not too surprising that also the field-dependent electrical conductivities of the Gaussian and the Nosé-Hoover thermostated Lorentz gas are not the same, as we have discussed in Sections III.B.4 and IV.C.3, see Figs. 7 and 11. Furthermore, even for Nosé-Hoover only the Lorentz gas conductivities still depend on the value for the coupling parameter between subsystem and reservoir, in the same way as the bifurcation diagrams of the different attractors.

On the other hand, all conductivities jointly exhibit a profoundly nonlinear response for the numerically accessible values of the field strength $\varepsilon > 0$. For the Gaussian thermostated Lorentz gas there must exist a regime of linear response in the limit of very small fields according to the mathematical proof by Chernov et al. However, the respective range of field strengths close to zero appears to be so small that up to now computer simulations could not really corroborate its existence. This reminds to some extent to van Kampen’s objections concerning the validity of linear response, who argued that a linear response is not trivially guaranteed for nonlinear chaotic dynamical systems. He emphasized that there might be a nontrivial interplay between microscopic nonlinearity and macroscopic linearity yielding a quantitatively negligibly small regime of linear response.

In addition to these problems concerning coarse functional forms, all field-dependent conductivities exhibit irregularities on fine scales that are not due to numerical errors. Such irregular transport coefficients are in fact well-known

⁴⁶In Ref. [Hoo98c] the phase space contraction at a stochastic boundary is defined by the second equation below Fig. 2. For this purpose an equality between phase space contraction and entropy production has been *stipulated* for this type of system. On the other hand, a natural assumption is just the conservation of phase space probability (or points in phase space) at the boundary, $dr'dv\rho(r,v) = dr'dv'\rho(r',v')$, where (r,v) represent position and velocity of a particle before a collision, (r',v') the same variables after a collision, and ρ is the respective probability distribution. A Jacobian at the collision is then straightforwardly defined by $|J| = |dr'dv'/drdv| = \rho(r,v)/\rho(r',v')$. If one follows this argument one arrives at the result of Ref. [Hoo98c] *only* (i) if both distributions before and after the collisions are identified with canonical distributions which is natural after a collision, but which is not so clear before a collision, cp., e.g., to Ref. [Wag99]; and (ii) if both distributions before and after a collision have precisely the same variance in terms of a temperature, $T = T'$. However, both distribution are only expected to be the same, with the same temperature, in the hydrodynamic limit, whereas systems of finite length as handled on the computer one may expect to exhibit temperature jumps [Kus02]. For this reason we consider the validity of the results reported in Refs. [Pos98,Pos00b] concerning the information dimension to be debatable.

from very related classes of dynamical systems, which share the properties of the periodic Lorentz gas of being deterministically chaotic, low-dimensional and spatially periodic. For very simple types of such systems it could be shown that these transport coefficients are even of a fractal nature. For thermostats of Nosé-Hoover type the irregularities appear to be smoothed-out, which may be understood with respect to the fact that here the kinetic energy fluctuates according to a canonical velocity distribution. Imposing instead a constant kinetic energy onto the system by means of a Gaussian thermostat these irregularities look considerably more “fractal-like”.

In summary, to us it still remains an open question to *quantitatively* identify a regime of linear response in the Gaussian thermostated driven periodic Lorentz gas, either analytically or numerically. One may furthermore ask whether such a regime of linear response may also be expected for applications of the Nosé-Hoover and possibly of other types of thermostats. On the other hand, one may suspect that the existence of irregularities on finer scales of the field-dependent conductivity is rather typical for deterministically thermostated driven periodic Lorentz gases. To which extend this holds true, and particularly how this goes together with the expected linear response for very small fields, are important open questions.

This points back again to the question concerning the equivalence of nonequilibrium ensembles. Unfortunately, in low-dimensional deterministic and periodic dynamical systems like the Lorentz gas the conductivity obviously reflects the specific type of thermal reservoir that has been applied. This appears to be at variance with such an equivalence that is expected to yield the same conductivities. Related findings have been reported in Ref. [Bon02]. In order to get more clear about this point it will be important to apply further types of thermal reservoirs to the Lorentz gas dynamics in order to check for similarities and differences, which we will do in the following two chapters.

Finally, as for the hotly debated fractality of attractors in NSS one may expect that the irregular or even fractal structure of parameter-dependent transport coefficients may be getting more regular by imposing stochasticity onto the system. This can be performed by either distributing the scatterers randomly in space, by using a stochastic thermal reservoir as discussed above, or by imposing additional noise onto a deterministic system. For thermostated driven *random* Lorentz gases field- and density-dependent Lyapunov exponents and diffusion coefficients have indeed already been calculated analytically and numerically [vB95,vB96,Lat97,Del97b,vB97,vB98,vB00b] verifying such a smooth dependence on parameters. Additionally, for simple low-dimensional maps it has been studied how the fractal structure of a parameter-dependent diffusion coefficient is affected while imposing different types of perturbations on them in time or in space [Kla02a,Kla02b]. As expected the fractality on arbitrarily fine scales disappears, however, irregularities still survive in form of smoothed-out oscillations. This irregular structure turns out to be very persistent against random perturbations, that is, typically rather strong random perturbations are needed to make the transport completely random walk-like.⁴⁷

Hence, there may be complicated scenarios between the two limiting cases of completely deterministic and completely stochastic diffusion, and the application of external randomness significantly affects fractal properties of the type as discussed above. Generally, one may expect that problems with linear response and the irregularity of parameter-dependent transport coefficients are rather specific to low-dimensional dynamical systems. For interacting many-particle systems, for example, it is natural to assume that all transport coefficients are smooth in their physical parameters and that there are broad regimes of linear response, as predicted by standard nonequilibrium thermodynamics. Examples of such systems will be discussed in Chapter VII.

F. Summary

1. Gaussian and Nosé-Hoover dynamics provide prominent examples for a non-Hamiltonian modeling of NSS. By employing the well-known baker map we demonstrated how volume-preserving “Hamiltonian” dynamics may go together with dissipative equations of motion and corresponding non-uniform probability densities. The key is the elimination of reservoir degrees of freedom by projecting out respective variables from the full equations of motion. Thus, there is nothing mysterious about using a non-Hamiltonian description of NSS.
2. Gaussian and Nosé-Hoover thermostats typically feature an identity between thermodynamic entropy production and the average rate of phase space contraction. However, there exists an even more general identity relating phase space contraction to entropy production in terms of the Gibbs entropy which is completely independent of the type of modeling. On the other hand, in case of a Hamiltonian approach to NSS the Gibbs entropy

⁴⁷An interesting exception is provided by a specific type of quenched disorder leading to a Golosov random walk. In this case an originally normal diffusive process may immediately become anomalous, that is, a diffusion coefficient does not exist anymore [Rad96].

production is simply zero. For this and other reasons one may doubt whether the Gibbs entropy should be considered as a correct definition of a nonequilibrium entropy being compatible with nonequilibrium irreversible thermodynamics.

Dissipative dynamical systems in NSS exhibit a negative average rate of phase space contraction. Due to the abovementioned identity the Gibbs entropy production is negative as well. This appears to be at variance with the second law of thermodynamics. However, here the Gibbs entropy can be saved by applying methods of coarse graining leading to an inversion of the sign.

To consider a coarse grained entropy production is furthermore suggested by the fact that the invariant measures of deterministically thermostated systems are typically singular. Still, the decisive question is whether the Gibbs entropy always yields the correct thermodynamic entropy production in nonequilibrium as, for example, compared to the Clausius entropy. For Gaussian and Nosé-Hoover thermostats this holds true, but there is no reason why this should generally apply to other types of thermal reservoirs.

3. Having an identity between phase space contraction and entropy production at hand enables one to link transport coefficients to dynamical systems quantities. Surprisingly, the escape rate approach to Hamiltonian dynamical systems yields a formula that is very analogous to the one obtained for dissipative dynamics: In both cases a transport coefficient is related to a difference between sums of Lyapunov exponents and the Kolmogorov-Sinai entropy on some fractal structure. In case of thermostated systems this structure consists of a fractal attractor, whereas for open Hamiltonian systems it is a fractal repeller.

There is even a third formula of a similar type derived for closed Hamiltonian dynamical systems, which connects the Hausdorff dimension of the hydrodynamic mode governing a transport process and a respective Lyapunov exponent to the corresponding transport coefficient. By performing suitable transformations the previous two formulas can be compared to the latter one. All resulting equations involve fractal dimensions of respective fractal sets and Lyapunov exponents thus revealing a striking formal analogy.

On the other hand, these equations are obtained from three very different approaches to NSS, and correspondingly the physical meaning of the involved quantities is rather different. We described a ‘master formula’ linking two of the three equations, however, its additivity suggests that there is no further reduction onto a common ‘root’. In addition, the formula derived for thermostated systems stands and falls with the validity of the identity between phase space contraction and entropy production, which in turn appears to be doubtful. In this respect the formulas emerging from the two Hamiltonian approaches seem to be on safer grounds.

4. We commented upon the suspected typicality of fractal attractors in dissipative NSS. For Gaussian and Nosé-Hoover thermostated systems there is a wealth of work corroborating the fractality of attractors. However, at least for the driven periodic Lorentz gas the topology of these fractal structures depends not only on the type of thermal reservoir used, but also on the variation of control parameters such as the coupling strength between subsystem and reservoir and the electric field strength. This is exemplified by bifurcation diagrams exhibiting complicated bifurcation scenarios for the attractor under variation of these parameters.

Alternatives to deterministic and time-reversible thermal reservoirs are provided by the stochastic Langevin equation and by stochastic boundary conditions. For a specific stochastically thermostated system it has been proven that the associated invariant measure is smooth hence contradicting the ubiquitous existence of fractal attractors in NSS. This was contrasted by numerical computations for other stochastically thermostated systems yielding again fractal objects, however, partly the numerical concepts employed appear to be debatable. Whether attractors in stochastically thermostated systems are typically smooth or fractal, or whether this actually depends on the specific type of system, remains an important open question.

5. A similar reasoning applies to the field-dependent conductivities of the thermostated driven periodic Lorentz gas. As in case of attractors, their functional forms reflects the specific type of thermal reservoir that has been applied. Numerically, no regimes of linear response could be detected for the driven periodic Lorentz gas, despite a proof for the existence of such a regime in the Gaussian thermostated case. In addition, all conductivities showed pronounced irregularities on finer scales as functions of the field strength which partly may be of a fractal origin. How the latter property goes together with a suspected linear response and to which extent all these properties hold for arbitrary thermal reservoirs remains to be clarified.

From a thermodynamic point of view these intricate dependencies of transport properties on parameter variations and on the type of reservoir are rather undesirable questioning the equivalence of nonequilibrium ensembles. One may thus attribute such nontrivial characteristics to the simplicity and low dimensionality of the model. This does not imply that the model itself is unphysical, since systems with these properties very well exist

in nature. Imposing randomness onto such dynamics indeed smoothes out these irregularities. Considering a higher-dimensional system composed of interacting many particles is expected to yield the same consequences.

In summary, a major question concerning the theory of transport in dissipative systems might be formulated as follows: How general are the results obtained from Gaussian and Nosé-Hoover thermostats for NSS of dissipative dynamical systems? That is, to which extent are these properties universal in that they hold for other thermostating schemes as well, or do they depend on the specific way of thermostating?

The remaining chapters of this review will be devoted to shed further light onto this fundamental question. Our approach will be carried out in two steps: A first step is to invent alternative, possibly more general thermostating schemes which are not fully identical to the previous class of methods but share certain characteristics with them, such as being deterministic and time-reversible and leading to NSS. In the following we present two generic examples of such methods. In a second step we study whether, by using these schemes, the same results for quantities characterizing chaos and transport are obtained as exemplified by Gaussian and Nosé-Hoover thermostats.

VI. GAUSSIAN AND NOSÉ-HOOVER THERMOSTATS REVISITED

In our previous discussions we have identified important crosslinks between chaos and transport in Gaussian and Nosé-Hoover thermostated models. Some authors even conjectured these relations to be universal for dissipative dynamical systems altogether. It is thus illuminating to look at simple generalizations of ordinary Gaussian and Nosé-Hoover dynamics, which we define again for the driven periodic Lorentz gas. We then analyze these thermostating schemes along the same lines as discussed previously, that is, by analytically and numerically studying the transport and dynamical systems properties of the respectively thermostated driven periodic Lorentz gas. Finally, we compare the results obtained from our analysis to the ones characterizing conventional Gaussian and Nosé-Hoover schemes as discussed in Chapters III to V.

A. Non-ideal Gaussian thermostat

Consider again the Gaussian thermostated driven periodic Lorentz gas defined by Eqs. (23), (26) with an external field that is parallel to the x direction, $\boldsymbol{\varepsilon} \equiv (\varepsilon_x, 0)^*$. We now distinguish between the interactions of subsystem and thermal reservoir parallel and perpendicular to the field direction by making the parallel coupling field-dependent,

$$\begin{aligned}\dot{r}_x &= v_x \\ \dot{v}_x &= \varepsilon_x - \alpha v_x - \alpha \varepsilon_x v_x \\ \dot{r}_y &= v_y \\ \dot{v}_y &= -\alpha v_y \quad ,\end{aligned}\tag{79}$$

where $\alpha \equiv \alpha(v_x, v_y)$. The difference to the Gaussian case is reminiscent by the third term on the right hand side of the second equation. This additional term conveniently adjusts the action of the thermostat to the anisotropy of the external field thus providing a physical justification for its introduction. Correspondingly, one may expect that this version thermalizes the driven Lorentz gas more efficiently than the conventional, as we may now call it, Gaussian thermostat Eqs. (23), (26). Formally, this generalization just amounts in making the conventional coupling constant field-dependent and then expanding it in the field strength ε_x in form of a power series, $\alpha \equiv (1 + \varepsilon_x)\alpha$. The conventional Gaussian case is obviously recovered in zeroth order while Eqs. (79) include the first order.

The explicit functional form for α can be calculated in complete analogy to Section III.A from the requirement of energy conservation yielding

$$\alpha(v_x, v_y) = \frac{\varepsilon_x v_x}{v^2 + \varepsilon_x v_x^2} \quad .\tag{80}$$

Comparing this result to the corresponding one for the conventional Gaussian thermostat Eq. (26) identifies the second term in the denominator as a new contribution. By using the definition of Eq. (27) the average phase space contraction rate is calculated to

$$\kappa = -\langle \alpha \rangle - \left\langle \frac{2\varepsilon_x^2 v_x v_y^2}{(v^2 + \varepsilon_x v_x^2)^2} \right\rangle \quad .\tag{81}$$

Again, a comparison of κ with the result for the conventional Gaussian thermostat Eq. (28) is instructive: apart from the correction already contained in α , Eq. (81) features a second term for the phase space contraction rate. All these additional terms become negligible in the limit of $\varepsilon_x \rightarrow 0$ thus approximately recovering the conventional Gaussian thermostat. But the point is that according to Eq. (81) there is clearly no identity between phase space contraction and thermodynamic entropy production anymore. Indeed, some entropy production related to Joule's heat, $dS = \varepsilon_x < v_x > /T$, see Eq. (30), is still reminiscent in Eqs. (80), (81), however, it does not show up in form of a simple functional relationship to the average phase space contraction rate.

We may thus refer to the coupling in terms of the conventional Gaussian thermostat defined by Eqs. (23), (26) as an *ideal coupling*, in the sense that it yields this simple identity, whereas we call the coupling Eqs. (79), (80) *non-ideal* in that it does not preserve the identity. Consequently, we call the thermostating scheme defined by Eqs. (79), (80) the *non-ideal Gaussian thermostat*.⁴⁸

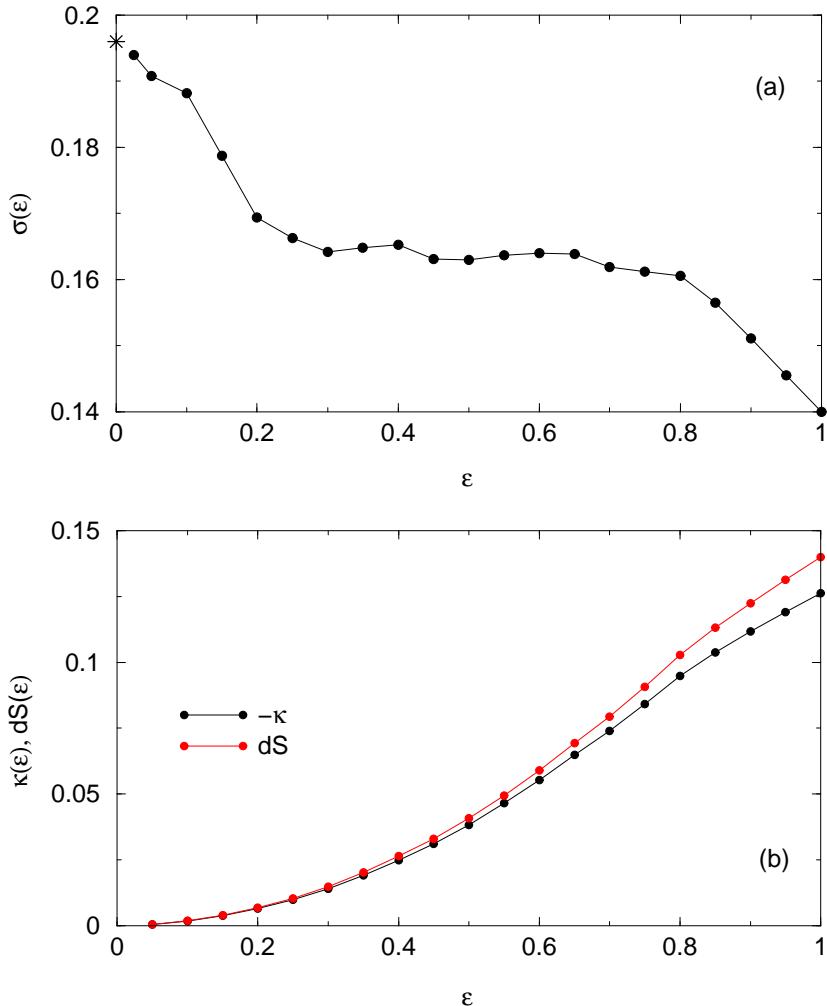


FIG. 13. Computer simulation results for the driven periodic Lorentz gas equipped with the non-ideal Gaussian thermostat Eqs. (79) at the temperature $T = 1$: (a) Field-dependent conductivity $\sigma(\varepsilon)$ as a function of the field strength $\varepsilon \equiv \varepsilon_y$. The star denotes the result in the limit of $\varepsilon \rightarrow 0$ according to the Einstein formula Eq. (34). (b) Comparison between the average phase space contraction rate $\kappa(\varepsilon)$ and the thermodynamic entropy production $dS(\varepsilon)$.

We now discuss computer simulation results for the driven periodic Lorentz gas thermostated that way [Kla99b]. Note

⁴⁸This scheme was orally presented on occasion of the conference on *Microscopic chaos and transport in many-particle systems* in Dresden, August 2002 [Kla].

that for technical reasons here the field of strength ε was chosen to be parallel to the y -axis, $\varepsilon \equiv \varepsilon_y$,⁴⁹ by adjusting the thermostating scheme in Eqs. (79) respectively. Fig. 13 (a) shows results for the conductivity $\sigma(\varepsilon)$ of the non-ideal Gaussian thermostated driven Lorentz gas. The fluctuations on small scales are less irregular than for the conductivity of the conventional Gaussian thermostat Fig. 7, which probably reflects the more efficient coupling with respect to the direction of the field. However, the oscillations seem to be less smooth than the ones for the Nosé-Hoover case shown in Fig. 11. Again there is no visible regime of linear response for $\varepsilon \rightarrow 0$. Curiously, the nonlinearities conspire to form an approximately linear response regime at intermediate values of the field strength; see, e.g., Ref. [Coh98] for a brief appreciation of such phenomena. Reassuringly, for small enough field strength the conductivity approaches the value indicated by a star, which was calculated from the respective diffusion coefficient in the field-free case according to the Einstein formula Eq. (34), see Section III.B.4.

Fig. 13 (b) depicts numerical results for the average phase space contraction rate Eq. (81) and for the thermodynamic entropy production according to $dS(\varepsilon) = \langle -\varepsilon v_y/v^2 \rangle = \sigma(\varepsilon)\varepsilon^2/T$. These results quantitatively confirm the non-identity between both quantities as already suggested by Eq. (81). Note that in analogy to the irregularity of $\sigma(\varepsilon)$ at least the entropy production $dS(\varepsilon)$ should yield irregularities on fine scales as well. However, this structure might be largely suppressed by the quadratic factor in ε . It would be interesting to investigate whether κ and dS exhibit different types of such irregularities corresponding to more intricate higher-order deviations between them.

Since there is no identity between phase space contraction and entropy production there is trivially no simple relation between the conductivity and the Lyapunov exponents such as the Lyapunov sum rule Eq. (33), cp. to its derivation for the conventional Gaussian thermostat in Section III.B.2. Indeed, for the average phase space contraction rate Eq. (81) it is not even obvious how to single out the conductivity without performing suitable approximations. For the two-dimensional Lorentz gas a conjugate pairing of Lyapunov exponents is guaranteed by default. However, one may conjecture that this property also holds in case of higher-dimensional non-ideal Gaussian thermostated systems. It is furthermore natural to assume that a fractal attractor exists for the respectively thermostated driven periodic Lorentz gas which is qualitatively of the same type as the one for the conventionally Gaussian thermostated model Fig. 5. These questions as well as how the respective non-ideal bifurcation scenario looks like remain to be investigated.

B. Non-ideal Nosé-Hoover thermostat

Precisely the same reasoning as for the non-ideal Gaussian thermostat can be applied for constructing a non-ideal Nosé-Hoover scheme. We illustrate this by summarizing results from Ref. [Rat00a]. Without loss of generality the coordinate system is chosen such that the direction of the field with strength ε is parallel to the x -axis. Indeed, with $\alpha \equiv (1 + \varepsilon_x)\alpha$ it is easy to see that the heuristic derivation for the conventional case provided in Section IV.B.1 must not be repeated, since all other functional forms remain precisely the same. This implies that even with a field-dependent α the respectively thermostated system is still transformed onto the same canonical distribution Eq. (42) as in case of the conventional Nosé-Hoover thermostat.

For our definition of the non-ideal Nosé-Hoover thermostat we thus simply combine Eqs. (79) with α defined by Eq. (44) yielding

$$\begin{aligned} \dot{r}_x &= v_x \\ \dot{v}_x &= \varepsilon_x - \alpha v_x - \alpha \varepsilon_x v_x \\ \dot{r}_y &= v_y \\ \dot{v}_y &= -\alpha v_y \\ \dot{\alpha} &= \frac{v^2 - 2T}{\tau^2 2T} . \end{aligned} \quad (82)$$

The conventional Nosé-Hoover thermostat Eqs. (23), (44) is recovered from these equations as a special case in thermal equilibrium, $\varepsilon_x \rightarrow 0$.

That the strength of the coupling between particle and reservoir is indeed properly adjusted to the anisotropy induced by the field is made more explicit as follows: Eqs. (82) can be rewritten by defining two field-dependent friction coefficients, $\alpha_x = (1 + \varepsilon_x)\alpha$ and $\alpha_y \equiv \alpha$, governed by

$$\dot{\alpha}_x = (v^2/2T - 1)(1 + \varepsilon_x)/\tau^2 \quad (83)$$

⁴⁹Numerical results indicated that for $\varepsilon||x$ the dynamics suffered from more creeping orbits than for $\varepsilon||y$.

and

$$\dot{\alpha}_y = (v^2/2T - 1)/\tau^2 \quad , \quad (84)$$

respectively. For each velocity component there is consequently a separate reservoir response time according to $\tau_x := \tau/\sqrt{1 + \varepsilon_x}$ and $\tau_y \equiv \tau$. Correspondingly, with increasing field strength the response time parallel to the field decreases thus making the action of the thermostat parallel to the field more efficient compared to the coupling perpendicular to the field.

In analogy to the previous section and to Sections III.B, IV.C, we shall now discuss the chaos and transport properties of the non-ideal Nosé-Hoover thermostated driven periodic Lorentz gas. Starting from Eq. (27) the phase space contraction rate of this thermostated system is obtained to

$$\kappa = -(2 + \varepsilon_x) < \alpha > \quad . \quad (85)$$

Performing an analogous calculation as in Section IV.C.1, i.e., starting from the energy balance Eq. (47) and requiring that the average time derivative of the total energy is zero, by using Eqs. (82) we arrive at the equation

$$\frac{\varepsilon_x < v_x >}{T} = 2 < \alpha > + \frac{\varepsilon_x < v_x^2 \alpha >}{T} \quad , \quad (86)$$

which should again be compared to the result of the conventional case Eq. (48). Obviously, as in case of the non-ideal Gaussian thermostat Eq. (81) there is a new second term that does not allow for an identity between the average phase space contraction rate and thermodynamic entropy production. In fact, if v_x^2 and α were independent quantities and if equipartition of energy were fulfilled, $< v_x^2 > = T$, then the identity would be recovered from Eq. (86). However, first of all, according to computer simulations v_x^2 and α are no independent quantities. Secondly, $< v_x^2 > = T$ is only strictly fulfilled in thermal equilibrium, thus the identity cannot hold.

Some numerical results for the phase space contraction rate κ and for the thermodynamic entropy production dS are presented in Table I at different values of τ and $\varepsilon \equiv \varepsilon_x$ yielding quantitative evidence for these deviations. An interesting aspect is that both functions apparently cross each other, which is at variance with the numerical results for the non-ideal Gaussian thermostat shown in Fig. 13, where $-\kappa$ appears to provide a lower bound for dS . The reason for this phenomenon is not yet understood and may deserve further investigations.

In analogy to the non-ideal Gaussian thermostat, Eq. (86) does not allow to recover the Lyapunov sum rule Eq. (51) as it holds for the conventional Nosé-Hoover thermostat: The electrical conductivity may be suitably introduced on the left hand side of Eq. (86), and by using Eq. (85) one may also replace the average friction coefficient in the first term on the right hand side by the average phase space contraction rate, respectively by the sum of Lyapunov exponents. Still, there remains the friction coefficient in the second term on the right hand side, which cannot be eliminated without making further assumptions. In any case, the resulting expression is significantly different from any ordinary Lyapunov sum rule as it holds for conventional Gaussian and Nosé-Hoover thermostats. Thus, the non-ideal Nosé-Hoover thermostat provides another counterexample against the universality of simple relations between chaos and transport in dissipative dynamical systems as discussed specifically in Section V.C.

No Lyapunov exponents have yet been computed for the non-ideal Nosé-Hoover thermostated driven periodic Lorentz gas. However, since this scheme defines also a bulk thermostat we would expect that conjugate pairing holds for the four Lyapunov exponents of this system.

In Section IV.C.2 we have outlined a generalized Hamiltonian formalism for the conventional Nosé-Hoover thermostat. Along similar lines a derivation for the non-ideal Nosé-Hoover thermostat can be performed [Kla]. The same holds for the non-ideal Gaussian thermostat in comparison to the conventional one. But these appear to be rather technical aspects such that we do not go into further detail here.

ε	$\tau = 1$		$\tau \simeq 31.6$	
	$-\kappa$	dS	$-\kappa$	dS
0.5	0.152	0.145	0.145	0.147
1.0	0.547	0.561	0.567	0.592
1.5	1.240	1.366	1.256	1.391

TABLE I. Average phase space contraction rate κ , see Eq. (85), and thermodynamic entropy production $dS = \varepsilon < v_x > /T$, $\varepsilon \equiv \varepsilon_x$, for the non-ideal Nosé-Hoover thermostated driven periodic Lorentz gas Eqs. (82). As a value for the temperature we have $T = 0.5$. The numerical error is about ± 0.001 . The data are from Ref. [Rat00a].

The structure of the attractor of the non-ideal Nosé-Hoover thermostated Lorentz gas, if projected onto Birkhoff coordinates, see Section III.B.3, is qualitatively more “smoothed out” than the one of the conventionally Gaussian thermostated version Fig. 5. On the other hand, it is still a bit more detailed than the one corresponding to the attractor of the conventional Nosé-Hoover thermostat Fig. 9. Here we do not show the attractor generated by Eqs. (82) but refer to Ref. [Rat00a] for a respective figure and for further details.

Instead, we present a bifurcation diagram for the non-ideal Nosé-Hoover thermostated driven periodic Lorentz gas. Fig. 14 may be compared to the one of the conventionally Nosé-Hoover thermostated case Fig. 10 (a). Although the response time τ is one order of magnitude smaller for the conventional case than for the non-ideal version thus indicating a more efficient coupling to the thermal reservoir, the action of the non-ideal version appears to be similarly efficient concerning a full covering of the phase space, which in both cases breaks down approximately at $\varepsilon \simeq 2$. This is in full agreement with the physical motivation for introducing the field-dependent coupling as discussed in the previous section in that it should enhance the efficiency of the thermostat’s action compared to conventional schemes. A bifurcation diagram for the conventional Nosé-Hoover case at $\tau = 1$ can be found in the material accompanying Ref. [Rat00a] and confirms our above assessment.

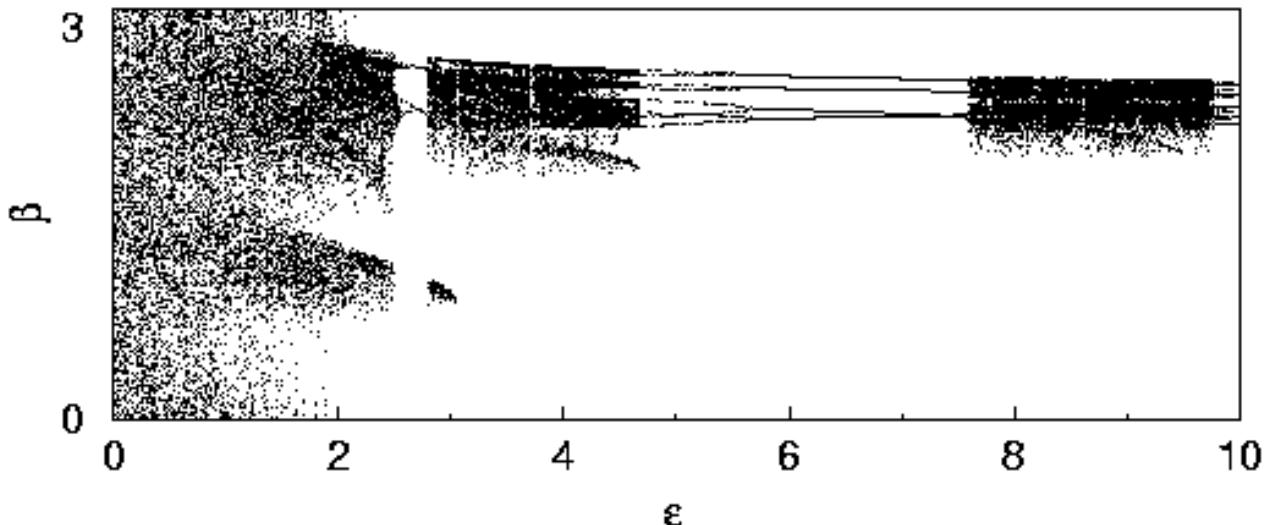


FIG. 14. Bifurcation diagram for the non-ideal Nosé-Hoover thermostated periodic Lorentz gas driven by an electric field of strength ε which is parallel to the x -axis. β is defined in Fig. 4. The temperature is $T = 0.5$, the reservoir coupling parameter $\tau = 1$. The figure is from Ref. [Rat00a].

The parameter-dependent electrical conductivity for the non-ideal version has not yet been computed, however, based on our discussion of the previous cases it is not unreasonable to expect that the results will just yield another highly nonlinear, irregular curve.

C. *Further alternatives to conventional Gaussian and Nosé-Hoover dynamics

In order to conclude this chapter we briefly summarize whether various mechanisms generating NSS fulfill the crucial identity between the average rate of phase space contraction and thermodynamic entropy production discussed before. To a large extent, these mechanisms have already been encountered on previous occasions, see in particular Sections IV.D and V.B.

Cohen and Rondoni showed that even the Gaussian *isoenergetic* thermostat applied to a many-particle system provides an identity between phase space contraction and entropy production only in the thermodynamic limit of a large number of particles [Coh98,Ron02a].

Benettin and Rondoni introduced a specific time-reversible rescaling of the single velocity components of a moving particle at the boundary of a system while keeping the total kinetic energy fixed [Ben01,Ron02a]. This mechanism may be considered as an intermediate case between a straightforward velocity rescaling, see Section III.A, and an ordinary Gaussian isokinetic thermostat. The complete dynamical system is defined such that it exhibits a symmetry breaking thus generating a current in a NSS. Similarly to the non-ideal thermostats discussed in the previous two sections, for small enough bias the average phase space contraction rate is getting proportional to the thermodynamic entropy

production while for larger bias this relationship becomes inherently nonlinear. Related dissipation mechanisms have been introduced earlier by Zhang and Zhang [Zha92] and in particular by Chernov and Lebowitz [Che95,Che97], see also Section VII.E.1 where we will discuss the example of a shear flow in a NSS. However, Chernov and Lebowitz argued for an identity according to their method.

As far as the generalized Nosé-Hoover thermostats sketched in Section IV.D are concerned, whether or not they exhibit an identity can easily be checked by following the second approach outlined in Section IV.C.1 for the example of the conventional Nosé-Hoover thermostat. It turns out that controlling higher even moments along the lines of Nosé-Hoover [Hoo89a,Jel89,Hoo96a,Pos97,Hoo97,Liu00], the Nosé-Hoover chain thermostat [Mar92b,Hoo97,Tuc00] and the deterministic formulation of a Langevin-like equation according to Bulgac and Kusnezov [Bul90b] all preserve the identity. These schemes are furthermore all time-reversible thus sharing fundamental properties with the class of conventional Gaussian and Nosé-Hoover thermostats.

The cubic coupling scheme proposed by Kusnezov et al. [Kus90,Bul90a], on the other hand, is time-reversible but does not show the identity. In this case the non-identity is due to a thermalization of the position coordinates creating an additional phase space contraction that does not contribute to an entropy production in terms of Joule's heat. In a way, this method exemplifies our assessment formulated in Section V.B that the phase space contraction of a dynamical system may involve contributions that, from the point of view of a thermodynamic entropy production, simply do not matter. Unfortunately, as we discussed already in Section IV.D.2 the physical interpretation of thermalizing position coordinates in the cubic coupling scheme remains rather unclear. Hence, this modeling may not be considered as an unambiguous counterexample concerning the identity.

The generalized Nosé-Hoover thermostats introduced by Hamilton et al. [Ham90,L'H93] and by Winkler et al. [Win92,Win95] are all time-reversible but do not fulfill the identity either. However, here it is not yet clear whether these schemes work conveniently in nonequilibrium situations. The methods proposed by Branka et al. [Bra00a,Bra00b] and by Sergi et al. [Ser01] are already not time-reversible and hence do not qualify as counterexamples for Gaussian and Nosé-Hoover dynamics.

Apart from considering the action of thermal reservoirs leading to dissipative dynamical systems we may recall that there are other ways in order to create NSS which do not involve any phase space contraction thus also providing counterexamples concerning an identity. For example, Gaspard studied diffusion under concentration gradients, respectively dynamical systems under flux boundary conditions [Gas97,Gas98a]. Eckmann et al. considered a model for a heat flow by using a fully Hamiltonian thermal reservoir consisting of infinitely many planar waves [Eck99a]. All these studies are reminiscent of the Hamiltonian approach to NSS. In the latter case the system actually reminds of the infinite Hamiltonian modeling of the Langevin equation, see Section II.B, rather than the thermostating approach. In any case, in both situations there is by default no phase space contraction and consequently no identity. Similarly, van Beijeren and Dorfman argued for a non-existence of this identity by using a Lorentz gas model for a heat flow [vB00a], however, their argument appears to be debatable.

Finally, Nicolis and Daems analyzed the general setting of dynamical systems perturbed by noise by deriving a balance equation for the entropy production [Nic96,Nic98,Dae99]. They found correction terms to an identity between phase space contraction and entropy production which they identified as functions of the noise strength. But in this case the dynamical systems considered are again not time-reversible anymore because of the noise and thus belong to a different class than conventional Gaussian and Nosé-Hoover thermostats.

D. Summary

1. We introduced a straightforward generalization of the conventional Gaussian thermostat, again for the example of the driven periodic Lorentz gas. This thermostating scheme is by default deterministic and time-reversible but is constructed such that it does not yield an identity between the average rate of phase space contraction and thermodynamic entropy production. We coined this method the *non-ideal Gaussian thermostat*. Since there is no identity there is also no Lyapunov sum rule relating transport coefficients to dynamical systems quantities. The field-dependent conductivity of this model is again highly nonlinear and different from the one found in other thermostated driven periodic Lorentz gases.
2. In the same vein, we introduced a *non-ideal Nosé-Hoover thermostat* that also does not exhibit the identity and hence no Lyapunov sum rule. In both cases, the non-identity resulted from modifying the coupling between subsystem and thermal reservoir by suitably adjusting it to the symmetry breaking caused by the external electric field. This even increased the efficiency of the non-ideal thermostats compared to their conventional colleagues as could be seen, for example, by means of matching bifurcation diagrams.

3. We finally summarized various other existing approaches towards the construction of NSS by inquiring whether or not they feature an identity between phase space contraction and entropy production. Apart from Hamiltonian modelings of NSS, it appears that there are many other examples of thermostating schemes not providing such an identity. However, in most cases they have not yet been studied respectively in nonequilibrium situations.

VII. STOCHASTIC AND DETERMINISTIC BOUNDARY THERMOSTATS

Gaussian and Nosé-Hoover schemes belong to the class of so-called *bulk thermostats*, that is, they remove energy from a subsystem during the originally free flight of a particle. *Boundary thermostats*, on the other hand, change the energy of a particle only at the collisions with the boundaries of the subsystem.⁵⁰

In this chapter we construct and analyze fundamental types of the latter class of thermostats. We start with well-known stochastic versions, which are so-called *stochastic boundary conditions* as they have already been mentioned in Section V.D. We then show how to make stochastic boundaries deterministic and time-reversible by using a simple chaotic map. This recent, new modeling of a thermal reservoir was called *thermostating by deterministic scattering* in the literature. The equations of motion resulting from this method are still deterministic and time-reversible hence sharing fundamental properties with Gaussian and Nosé-Hoover schemes. However, both the construction of this deterministic boundary thermostat and the dynamics associated with it are generally very different in comparison to conventional bulk thermostats.

An analysis of models thermostated by deterministic scattering thus enables us to learn more about possible universal properties of nonequilibrium steady states in dissipative dynamical systems. We demonstrate this by studying again the transport and dynamical systems properties of a respectively thermostated driven periodic Lorentz gas. Our findings are compared to the ones reported previously for Gaussian and Nosé-Hoover thermostats. We finally briefly discuss results for a hard-disk fluid under nonequilibrium conditions, which is also thermostated at the boundaries.

A. Stochastic boundary thermostats

Let us consider a point particle moving in a plane, which interacts with a thermal reservoir through collisions at a flat wall, see Fig. 15. If the reservoir is in thermal equilibrium at a certain temperature, the reservoir degrees of freedom will be distributed according to a canonical distribution. Consequently, the subsystem particle will be thermalized at the collision with respect to a Gaussian velocity distribution. If we assume that the memory of the particle is completely lost at the collision, the velocity after the collision can be randomly sampled from the respective velocity distribution of the thermal reservoir. This is the physical essence of what is called *stochastic boundary conditions*, see also our brief account of them in Section V.D.

Casting this physical picture into an equation it must be taken into account that an impenetrable wall breaks the symmetry of the subsystem. That is, there are different velocity distributions parallel and perpendicular to the wall: Parallel to the wall the particle's outgoing velocity component v'_x , see Fig. 15, should be sampled simply from the Gaussian distribution for reservoir velocities parallel to the wall. However, in the perpendicular direction an observer who is sitting at the wall will measure a non-zero average flux of reservoir, respectively subsystem particles to the wall. This flux is due to the fact that all these particles can approach the impenetrable wall from one side only. Consequently, the symmetry of the corresponding distributions of velocity components perpendicular to the wall is broken as well. This is properly modeled by multiplying the bulk velocity distribution of reservoir, respectively subsystem, with the absolute value of the perpendicular velocity component, $|v_y|$.

In summary, if the velocity distribution of the thermal reservoir is canonical at temperature T an observer at the boundary measures for the two velocity components $v_x \in [-\infty, \infty)$, $v_y \in [0, \infty)$ of a reservoir particle colliding with the boundary [Leb78,Cic80,Ten82,Che95,Che97,Wag99]

$$\rho(v_x, v_y) = (2\pi T^3)^{-1/2} |v_y| \exp\left(-\frac{v_x^2 + v_y^2}{2T}\right) . \quad (87)$$

⁵⁰Of course, the action of Gaussian and Nosé-Hoover thermostats can be restricted to some boundary layers of a subsystem thus bridging the gap between bulk and boundary thermostats as has been done in Ref. [Pos89].

The subsystem particle must then exhibit precisely the same distribution of outgoing velocities, under the conditions that its velocities before and after the collision are not correlated and that the reservoir distribution is not modified.

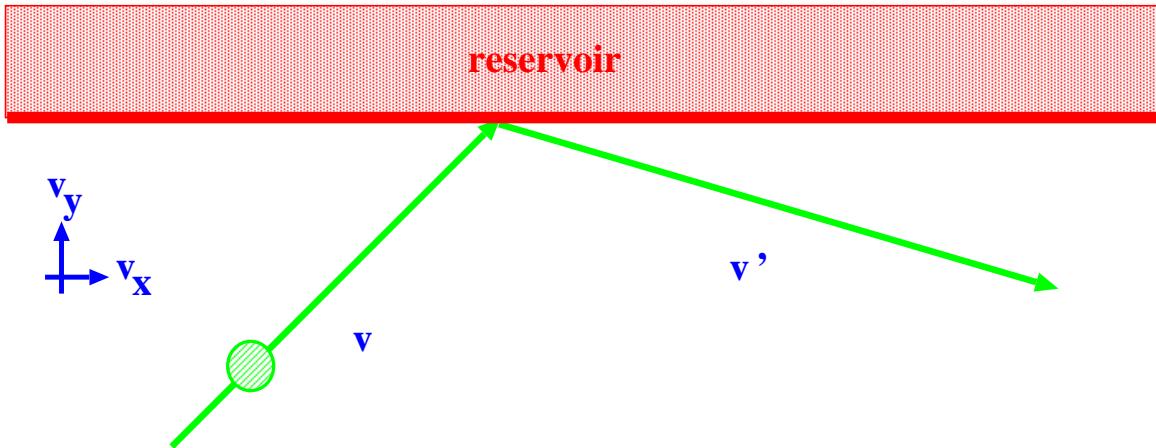


FIG. 15. Setup for defining stochastic boundary conditions: a point particle of mass $m = 1$ moving with velocity \mathbf{v} collides inelastically with a flat wall. The velocity after the collision is denoted by \mathbf{v}' . The difference in the kinetic energy $(v'^2 - v^2)/2$ is transferred to, or from, a thermal reservoir associated with the wall. \mathbf{v}' is obtained according to Eq. (89), see the text.

In practice, these scattering rules are implemented as follows [Wag99]: draw two independently and identically distributed random numbers $\zeta, \xi \in [0, 1]$ from a uniform density $\rho(\zeta, \xi) = 1$ by using a suitable random number generator. The transformation rules of how to get from these uniform distributions to the Gaussian ones of Eq. (87) can be calculated from the requirement of phase space conservation.⁵¹ For the outgoing velocities $v'_x, v'_y \in [0, \infty)$ this condition reads

$$\begin{aligned} \rho(\zeta)\rho(\xi) \left| \frac{d\zeta d\xi}{dv'_x dv'_y} \right| &= \sqrt{\frac{2}{\pi T^3}} |v'_y| \exp\left(-\frac{v'^2_x + v'^2_y}{2T}\right) \\ &= \left| \frac{\partial \mathcal{T}(v'_x, v'_y)}{\partial v'_x \partial v'_y} \right| . \end{aligned} \quad (88)$$

Integration yields for the transformation \mathcal{T} the functional form

$$\begin{aligned} (v'_x, v'_y) &= \mathcal{T}^{-1}(\zeta, \xi) \\ &= \sqrt{2T} \left(\text{erf}^{-1}(\zeta), \sqrt{-\ln(\xi)} \right) , \end{aligned} \quad (89)$$

which completes the algorithm.

B. Deterministic boundary thermostats, or thermostating by deterministic scattering

From the point of view of dynamical systems theory the problem with stochastic boundaries is that they are not deterministic and time-reversible. Consequently, they do not enable a detailed analysis of transport and dynamical systems properties of dissipative systems as outlined in the previous chapters. However, this problem can rather straightforwardly be resolved as follows [Kla00b, Rat00b, Wag99]: Let $\mathcal{M} : [0, 1] \rightarrow [0, 1], (\zeta, \xi) \mapsto \mathcal{M}(\zeta, \xi)$ be a two-dimensional deterministic map with an inverse \mathcal{M}^{-1} . Loosely speaking, the random number generators in Eq. (89) are then replaced by the action of this map, however, in form of the following scattering rules

$$(|v'_x|, |v'_y|) = \begin{cases} \mathcal{T}^{-1} \circ \mathcal{M} \circ \mathcal{T} (|v_x|, |v_y|) & ; v_x \geq 0 \\ \mathcal{T}^{-1} \circ \mathcal{M}^{-1} \circ \mathcal{T} (|v_x|, |v_y|) & ; v_x < 0 \end{cases} \quad (90)$$

⁵¹For a two-dimensional Gaussian without a flux term the same reasoning in polar coordinates leads to the well-known Box-Müller algorithm [Pre92].

with $\mathcal{T}^{-1} : [0, 1] \times [0, 1] \rightarrow [0, \infty) \times [0, \infty)$. This prescription is not yet complete. First of all, we have to further specify the sign of the outgoing velocities. We do this for the geometry presented in Fig. 15 by requiring that particles going in with positive (negative) tangential velocity go out with positive (negative) tangential velocity. For the perpendicular component we require that v_y always changes its sign. This distinction between positive and negative velocities, supplemented by the respective use of \mathcal{M} and \mathcal{M}^{-1} in the equations, renders the collision process time-reversible. This is easily verified by using the collision rules Eq. (90) and reversing the direction of time after a collision. Finally, to avoid any artificial symmetry breaking in numerical experiments, the application of \mathcal{M} and \mathcal{M}^{-1} in Eq. (90) should be alternated with respect to the position of the scattering process at the wall.

It remains to characterize the map \mathcal{M} of this equation in more detail. In order to compare with Gaussian and Nosé-Hoover thermostats we require that this map is deterministic and reversible; for a definition of the latter property see footnote number 36. Furthermore, \mathcal{M} should be mixing [Arn68,Sch89,Gas98a,Dor99] implying ergodicity and, under rather general conditions, also chaotic behavior [Dev89,Ban92] in the sense of exhibiting a positive Lyapunov exponent [Ott93]. Preferably, the map should also be uniformly hyperbolic [Eck85,Ott93,Gas98a,Dor99], and for convenience it should generate a uniform probability density in phase space. All these properties, except the last one, are necessary conditions for enabling a proper thermostating. That is, the whole phase space of the map should be sampled such that, in combination with the transformation \mathcal{T} according to Eq. (90), the canonical distribution can be reproduced completely on the basis of these scattering events; see also Section IV.D.1 for a related discussion of necessary conditions regarding a proper functioning of deterministic thermostats.

Apart from these constraints the precise functional form of the map appears to be arbitrary. By choosing different maps one may model different particle-wall interactions. In this respect the map \mathcal{M} together with the transformation \mathcal{T} plays the role of a scattering function containing detailed information about the microscopic scattering process of a particle. Fixing the functional form of the map completes our set of scattering rules, which has been called *thermostating by deterministic scattering* [Kla00b,Rat00b,Wag99,Rat02].

If not indicated otherwise, in the following we will choose for \mathcal{M} the probably most simple example of a map fulfilling all of the above requirements. This is the two-dimensional *baker map* as it has been introduced and explicitly discussed in Section V.A, see Eq. (58) and the corresponding Fig. 12. However, we remark that other simple maps such as the cat map, respectively for general values of the control parameter the sawtooth map, as well as the standard map [Sch89,Ott93,Mei92,All97], both for large enough values of their control parameters, have also been used within this scheme already [Wag99,Kla99b,Wag00].

C. *Stochastic and deterministic boundary thermostats from first principles

There are two crucial ingredients in the approach outlined above leading to stochastic and deterministic boundary thermostats: Firstly, the knowledge of the equilibrium velocity distribution functions of a thermal reservoir with infinitely many degrees of freedom is required. Secondly, the energy transfer at the boundaries must be defined in form of suitable microscopic collision rules.

In both respects specifically our derivation of thermostating by deterministic scattering is quite heuristic. That is, we started from essentially pre-defined stochastic boundaries and conveniently modified them by choosing new collision rules. However, a systematic construction from first principles should rather proceed the other way around by first leading to the general solution, which is the deterministic case, and then recovering the stochastic case by eliminating any correlations at the collisions with the wall. Such an approach should provide more insight into the detailed mechanism and into the conditions for a proper functioning of this thermostat. Here we outline in three steps how such a systematic construction is performed [Kla00b,Rat00b]:

1. equilibrium velocity distribution functions:

Our first goal is to construct a model for a thermal reservoir consisting of an arbitrary but finite number of degrees of freedom. For this purpose we need to know the velocity distribution functions of a subsystem consisting of d_s degrees of freedom, which interacts with a thermal reservoir of $d_r < \infty$ degrees of freedom in thermal equilibrium. With $d = d_s + d_r$ we denote the total number of degrees of freedom, where $d_s < d_r$, and we may assume that there is only kinetic energy. In Section II.C we have summarized how to calculate the finite-dimensional velocity distributions of the subsystem by giving some exact results; see Eq. (19) for the equilibrium distribution of one velocity component v_1 and Eq. (20) for the distribution of the absolute value of the velocity vector of two components v_1 and v_2 with $v = \sqrt{v_1^2 + v_2^2}$.

Note that the corresponding distribution functions are bulk distributions only, whereas, for defining a boundary thermostat, we need to know the functional forms of these distributions at the boundaries of the thermal reservoir, respectively of the subsystem. This bulk-boundary transformation may be performed heuristically such as outlined

in the previous section. Ref. [Rat00b] provides a more microscopic derivation of this relation by means of calculating the average time of flight between two collisions and the average collision length. In any case, all these arguments eventually amount in a multiplication of the finite-dimensional bulk densities Eqs. (19), (20) with a “flux” factor of v_1 , respectively of v , supplemented by a suitable renormalization of the associated velocity distributions.

2. defining a proper coupling:

Knowing these fundamental functional forms of the subsystem’s boundary equilibrium velocity distribution functions, the next step is to define a suitable microscopic coupling between subsystem and thermal reservoir. The coupling should be such that it establishes an energy transfer between subsystem and reservoir degrees of freedom, which generates the desired velocity distribution. In order to preserve the Hamiltonian character of the microscopic equations of motion of the subsystem to be thermostated we demand that this coupling is deterministic and time-reversible. In some sense, there should furthermore be conservation of phase space volume, as will be explained later on.

A first idea of how such a coupling may look like can be obtained from the *rotating disk model*: Let us consider a unit cell of the field-free periodic Lorentz gas, see the geometry of Fig. 3, where the fixed disk rotates with an angular velocity ω . Altogether we have thus three degrees of freedom, two for the moving point particle and one for the rotating disk. Assuming that the particle is elastically reflected perpendicular to the disk reduces the problem of an energy transfer between particle and disk to the problem of two elastically colliding masses on a line. The corresponding equations of motion can easily be derived and are of the form of a nonlinear two-dimensional map governing the exchange between translational and rotational energy.

This rotating disk model was originally proposed in Ref. [Rat00b] but became more popular only later on by applying it to a periodic Lorentz gas under a temperature gradient, see Ref. [MM01] and more recent studies in Refs. [Lar03,Bun03]. Here all disks of the spatially extended Lorentz gas rotate with different angular velocities thus mimicking a thermal reservoir of, in principle, arbitrary dimensionality. Interactions between these different rotational degrees of freedom are provided by the moving particle carrying energy from one disk to another. To some extent, this Hamiltonian modeling of a thermal reservoir reminds of the one employing an arbitrary number of harmonic oscillators which was used for deriving the stochastic Langevin equation, see Section II.B. It thus suffers from the same deficiency that, at least numerically, it cannot conveniently be applied to nonequilibrium situations involving external fields, because in this case an infinite number of reservoir degrees of freedom is needed in order to continuously remove energy from the subsystem.

Hence we follow a different path leading to a more abstract and more general model of a thermal reservoir. This approach is further motivated by a second problem with the rotating disk model: Computer simulations for a single rotating disk under periodic boundary conditions show that only for specific values of the associated control parameters this coupling reproduces the equilibrium velocity distributions Eqs. (19), (20) at $d = 3$ [Rat00b,Lar03]. This reflects the fact that generally the dynamics of this system is very complicated indicating non-ergodic behavior in a mixed phase space consisting of islands of stability and chaotic layers. As a consequence, not for all values of the control parameters there is equipartitioning of energy, which is needed for a microcanonical distribution for subsystem plus thermal reservoir [Rei65]. In turn, only the presence of equipartitioning appears to guarantee a proper energy transfer between subsystem and reservoir degrees of freedom providing a proper thermalization.

In other words, an arbitrary map \mathcal{M} defining the collision rules of a moving particle with a disk, such as provided by the rotating disk model, must generally be *enforced* to yield equipartitioning of energy, respectively the desired equilibrium velocity distributions for reservoir and subsystem.⁵² This can be achieved by, first of all, choosing a map \mathcal{M} that is sufficiently ‘nice’, in the sense of fulfilling the list of necessary conditions already provided in the previous section. The map must further be combined with a second map \mathcal{T} according to Eq. (90) in order to ensure that the desired functional forms of the equilibrium velocity distributions are attained. This map \mathcal{T} is defined in complete formal analogy to Eqs. (88), (89) in replacing the Gaussian of Eq. (88) by the finite-dimensional “target” velocity distribution function determined by Eq. (19).

As an example, let us consider a single Lorentz gas scatterer under periodic boundary conditions. We modify the collision rules according to the above reasoning such that this system mimicks a rotating disk-like situation with $d_s = 2$ for the moving particle and $d_r = 1$ associated with the disk, thus $d = 3$ altogether. For the map \mathcal{M} we choose again the baker map Eq. (58). The target equilibrium velocity distributions are determined by Eqs. (19), (20) at $d = 3$. The transformation \mathcal{T} is then calculated from the prescription used in Eq. (88) if the Gaussian of this equation is replaced by the respective functions of Eqs. (19), (20) at $d = 3$. Here one needs to make a choice concerning the coordinate system in which the velocity variables shall be defined. For the Lorentz gas disk one may choose, e.g., a

⁵²In Ref. [Lar03] it was argued that relating different rotational degrees of freedom to different disks also resolves this problem.

local coordinate system with respect to the point at the collision. Some further details are explained in the following section. The resulting expression for \mathcal{T} is finally combined with the map \mathcal{M} according to Eq. (90). Computer simulations of this inelastic Lorentz gas scatterer provide evidence that, indeed, the desired velocity distributions are generated by this model [Rat00b].

Obviously, the general idea underlying this method is not restricted to $d = 3$. According to the transformation \mathcal{T} , all what we need to know is the proper equilibrium distribution function of a thermal reservoir associated with d_r degrees of freedom while interacting with a subsystem of d_s degrees of freedom. In other words, we do not need to care about any explicit equations of motion defining d_r degrees of freedom in order to model a thermal reservoir. From now on we therefore carefully distinguish between the *number of degrees of freedom* of the thermal reservoir that we mimick, and the *number of dynamical variables* which are actually involved in modeling this reservoir. For the collision rules that we are currently discussing the action of the thermal reservoir may be represented by one dynamical variable only: Let k represent the absolute value of the velocity vector of all reservoir degrees of freedom. The value of k is then defined via energy conservation for subsystem plus reservoir, $E = v^2/2 + k^2/2$, where v is the absolute value of the velocity of a subsystem particle before a collision. Accordingly, the value v' after a collision is generated by the collision rules Eq. (90), with a suitable choice for \mathcal{T} , and the corresponding value k' of the reservoir variable is again obtained from energy conservation. Thus, $\Delta k := k' - k$ yields the energy transfer between subsystem and reservoir at a collision.

We add that this general formalism might be used to obtain deterministic and time-reversible collision rules for two colliding granular particles instead of using normal and tangential restitution coefficients according to which the microscopic dynamics is dissipative, non-Hamiltonian, and not reversible. A finite-dimensional thermal reservoir then mimicks d_r internal degrees of freedom of some granular material storing kinetic energy from which it can be restored at a collision, compare, e.g., to microscopic models of inelastic collisions as discussed in Refs. [Asp98,Bri96]. However, note that we did not yet arrive at the transformation represented by Eq. (89), since our collision rules still concern a finite dimensional thermal reservoir only.

3. modeling an infinite dimensional reservoir:

In a general nonequilibrium situation only a thermal reservoir consisting of an infinite number of degrees of freedom is able to continuously absorb energy and to possibly generate a NSS. For the equilibrium velocity distributions Eqs. (19), (20) this implies that we need to take the limit of $d \rightarrow \infty$. As was shown in Section II.C, employing equipartitioning of energy we then arrive at the well-known canonical distributions Eqs. (21), (22). In this limit the total energy of the thermal reservoir is not well-defined anymore, consequently it cannot be represented by a dynamical variable k as introduced for the finite-dimensional case discussed above. However, this variable can easily be dropped, since it does not appear explicitly in the collision rules.

By using now the canonical velocity distribution Eq. (21) we arrive at Eq. (88) in order to define the transformation \mathcal{T} . Neglecting any correlations in the map \mathcal{M} before and after a collision, the stochastic boundary conditions Eqs. (89) are recovered from their deterministic counterpart Eq. (90) as a special case. Hence, we may say that this approach provides a derivation of stochastic boundaries from first principles. In fact, thermostating by deterministic scattering was first constructed by following this bottom-up approach [Kla00b,Rat00b]. Only subsequently it was realized that the final outcome may be considered as a deterministic generalization of stochastic boundaries along the top-to-bottom approach of Section VII.A [Wag99]. This completes our derivation of a modeling of stochastic and deterministic boundaries “from first principles”.

We conclude this section by taking up the thread from Sections II.C and V.A, in which we provided a simple explanation for the origin of an average phase space contraction in thermostated nonequilibrium systems. In fact, the previous bottom-up approach towards deterministic boundary thermostats nicely illustrates the respective reasoning as follows: Let us start in an equilibrium situation with constant total energy and let the number $d = d_s + d_r$ of degrees of freedom of subsystem plus thermal reservoir for a moment again be finite. As we explained in Section II.C, in this case an ensemble of points representing the combination of subsystem plus reservoir is uniformly distributed on a hypersphere in velocity space indicating that there is no average phase space contraction. However, the projected-out velocity distributions of the subsystem are typically not uniform anymore, cp. to Eqs. (19), (20).

Correspondingly, by calculating the Jacobian determinant for the collision rules Eqs. (90) *only* on the basis of respective functional forms of \mathcal{T} for given d , one finds that the subsystem dynamics alone is not phase space conserving at a single collision [Kla]. This should not come as a surprise, since at any collision there is an exchange of kinetic energy with the reservoir. Nevertheless, in case of an equilibrium situation the *average* phase space contraction rate for the subsystem is still zero reflecting the fact that on average there is no energy transfer between subsystem and reservoir. This was also confirmed numerically for the respectively modified Lorentz gas.

The apparent phase space contraction at a collision simply results from the fact that so far we looked at the dynamics of the subsystem only. In a complete analysis the dynamics of the thermal reservoir must be taken into account

as well. This dynamics is adequately represented by the variable k , which, here, is well-defined again because of $d < \infty$ and can be obtained via energy conservation. The complete dynamics thus actually consists of the set of variables (\mathbf{v}, k) . By looking at the Jacobian determinant of the combined system (\mathbf{v}, k) one can indeed verify that the complete dynamics is always locally phase space conserving. Consequently, there is no contradiction between a locally dissipative dynamics of the subsystem alone and a phase space preserving Hamiltonian character of the full equations of motion for subsystem plus thermal reservoir.

Let us now apply these arguments to a nonequilibrium situation, e.g., by imposing an external field onto the subsystem. The field will continuously increase the kinetic energy of a particle moving in the subsystem, and the thermal reservoir will continuously absorb this energy through collisions by storing it onto infinitely many degrees of freedom according to equipartitioning of energy. During the free flight of the particle there is no action of the thermal reservoir, and the subsystem is trivially Hamiltonian. At a collision we are using precisely the same collision rules as defined above for which we have argued, in case of $d < \infty$, that there is no loss of phase space volume either. Consequently, by properly looking at subsystem *plus* thermal reservoir we conclude that the whole dynamics is phase space conserving, and in this respect Hamiltonian-like, in nonequilibrium as well. This is not in contradiction to the fact that there is an average flux of energy from the subsystem to the thermal reservoir, which counterbalances the generation of an average current parallel to the external field. These arguments should also be valid by making the number of reservoir degrees of freedom arbitrarily large, that is, in the limit of $d \rightarrow \infty$.

We finally remark that, although for thermostating by deterministic scattering the equations of motion appear to be compatible with a Hamiltonian dynamics, as argued above, a Hamiltonian formulation of this scheme is currently not known.

D. Deterministic boundary thermostats for the driven periodic Lorentz gas

Let us now apply the scheme of thermostating by deterministic scattering to the periodic Lorentz gas by modeling a thermal reservoir mimicking an *infinite number* of degrees of freedom as outlined in the previous section. That is, the originally elastic collisions of the moving particle with the hard disk are made *inelastic* allowing for an energy transfer at a collision without changing the geometry of the system. Note that the unit cell with a single scatterer is periodically continued by applying periodic boundary conditions. In physical terms one may thus think of the arbitrarily many degrees of freedom that we are now going to associate with the disk as mimicking, e.g., different lattice modes in a crystal, which remove energy from a colliding particle.

This modification of the standard Lorentz gas is performed by adapting the collision rules Eqs. (58), (89) and (90) to the circular geometry of a Lorentz gas disk. For this purpose we replace the usual Cartesian coordinates by the tangential, respectively the normal component of the velocity of the colliding particle in a local coordinate system at the scattering point. That is, we write $v_{\parallel} \equiv v_x$ and $v_{\perp} \equiv v_y$ in Eqs. (89), (90). Alternatively, one may wish to choose local polar coordinates [Kla00b,Rat00b].

We are now prepared to study the chaos and transport properties of the driven periodic Lorentz gas thermostated by deterministic scattering and to compare the results with the previous ones obtained for ideal and non-ideal Gaussian and Nosé-Hoover thermostats. Note that thermostating by deterministic scattering was constructed in order to generate a canonical velocity distribution in thermal equilibrium. In this respect this boundary thermostat forms a counterpart to the Nosé-Hoover thermostat acting in the bulk. In fact, our previous Fig. 8 depicts some representative nonequilibrium velocity distribution functions for the driven periodic Lorentz gas thermostated both by Nosé-Hoover and by deterministic scattering. For moderate to large response times the Nosé-Hoover distributions are indeed very similar to the one obtained from thermostating by deterministic scattering.

Concerning other chaos and transport properties we will show in the following that a comparison is more non-trivial. First we check analytically for an identity between phase space contraction and entropy contraction. We then show numerical results for the attractor both resulting from deterministic and from stochastic boundary thermostats. In the deterministic case we further discuss the associated bifurcation diagram as well as the electrical conductivity. Finally, we elaborate on the spectrum of Lyapunov exponents. In this section we particularly summarize results published in Refs. [Kla00b,Rat00b,Rat02].

1. Phase space contraction and entropy production

In contrast to bulk thermostats such as Gauss or Nosé-Hoover, for a driven periodic Lorentz gas thermostated at the boundaries the phase space volume is conserved during free flights between collisions. As was briefly mentioned in the previous section, any phase space contraction can thus only be generated by the collision rules defined in terms of

the composition of maps Eqs. (58), (89) and (90). For maps any change of the phase space volume is assessed by the Jacobi determinant, see Section V.A. In case of thermostating by deterministic scattering adapted to the Lorentz gas geometry this quantity may be denoted by $|dv'_{\parallel} dv'_{\perp}| / |dv_{\parallel} dv_{\perp}|$. Here the numerator is composed of the two velocity components after a collision and in the denominator there are the corresponding velocity components before a collision with the disk. If a particle collides $n \in \mathbb{N}$ times the product of Jacobian determinants evolves in time according to

$$\prod_{i=1}^n \frac{|dv'_{i,\parallel} dv'_{i,\perp}|}{|dv_{i,\parallel} dv_{i,\perp}|} \equiv \exp \left(\sum_{i=1}^n \ln \frac{|dv'_{i,\parallel} dv'_{i,\perp}|}{|dv_{i,\parallel} dv_{i,\perp}|} \right) = \exp \left(n < \ln \frac{|dv'_{\parallel} dv'_{\perp}|}{|dv_{\parallel} dv_{\perp}|} > \right) . \quad (91)$$

For the last step it was assumed that the system is ergodic, which enables to replace the time average by an ensemble average over colliding particles. In this expression

$$\kappa_b := < \ln \frac{|dv'_{\parallel} dv'_{\perp}|}{|dv_{\parallel} dv_{\perp}|} > \quad (92)$$

is denoted as the average exponential rate of phase space contraction per unit time, where the index b indicates the definition at a boundary. This quantity is obviously zero if the map is volume preserving and deviates from zero otherwise. Hence, for time-discrete dynamics such as the collision map Eq. (90) under consideration κ_b replaces the average phase space contraction rate κ of time-continuous dynamics defined by Eq. (27).⁵³

For the periodic Lorentz gas thermostated by deterministic scattering κ_b can be calculated from the collision rules Eqs. (58), (89) and (90) to [Rat02]

$$\kappa_b = \frac{< v'^2 > - < v^2 >}{2T} , \quad (93)$$

where v' and v are the absolute values of the velocities after and before a collision, respectively. κ_b is thus identical to minus the average outward flux of kinetic energy to the reservoir $dQ := (< v^2 > - < v'^2 >)/2$ divided by the temperature T , where T derives from Eq. (89). This result holds in equilibrium as well as in nonequilibrium. As in case of Gaussian and Nosé-Hoover thermostats, Eq. (93) may now be compared to the entropy production $dS = dQ/T_r$ in terms of the heat transfer between subsystem and thermal reservoir, cp. to Section III.B.1, where T_r denotes the temperature of the thermal reservoir, leading to

$$\kappa_b = - \frac{T_r}{T} dS . \quad (94)$$

In this case, the question concerning an identity between dS and κ_b boils down to the problem whether the temperature T coming from Eq. (89) can always be identified with the actual temperature of the thermal reservoir T_r . In equilibrium, that is, without applying an external field ε , it is $T = T_r$ for the periodic Lorentz gas, which follows from the definition of this thermostating scheme outlined in Section VII.A to C. However, in this situation Eq. (94) is trivially zero on both sides anyway.

On the other hand, to define a proper temperature in a nonequilibrium situation is very problematic, see also our brief discussion in Section II.A. For our model one can argue at least along two different lines in order to define a proper reservoir temperature: One reasoning is that the temperature of a thermal reservoir consisting of an infinite number of degrees of freedom should never change under whatsoever nonequilibrium conditions and, hence, should always be the same as in thermal equilibrium [Hoo02a]. This implies $T_r \equiv T$ and according to Eq. (94) the identity between phase space contraction and entropy production, as discussed for ideal Gaussian and Nosé-Hoover thermostats, holds as well.

However, for all thermostats analyzed in this review it is well-known that generally the nonequilibrium temperature of the subsystem, if defined via the kinetic energy of the moving particle on the basis of equipartitioning of energy,

⁵³More explicitly, κ_b naturally shows up in the formal solution for the probability distribution function of the time-discrete Liouville (Frobenius-Perron) equation in dissipative maps. This is in full analogy to solving the time-continuous Liouville equation Eq. (37), where the average of the divergence plays the same role.

is not necessarily equal to the equilibrium reservoir temperature T that is contained in the equations of motion [Pos88, Pos89, Eva90b, Sea98, Rat00a]. In case of boundary thermostats this implies that identifying T_r with T typically yields temperature jumps at the boundaries [Kus02]. Such discontinuities in the temperature profile are at variance with a local equipartitioning of energy between the reservoir degrees of freedom and the degrees of freedom of the colliding particle.

In contrast to the first definition outlined above, this motivates to simply *assume* such an existence of a local equipartitioning of energy in a NSS. Under this assumption the reservoir temperature can be defined by computing the average kinetic energy of a particle at the moment of the collision [Wag99, Kla00b, Rat00b, Rat02]. This definition of a nonequilibrium temperature thus amounts in smoothly extrapolating the temperature profile from the bulk of the subsystem to the boundary of the reservoir. An application of this method to the boundary thermostated driven periodic Lorentz gas yields $T_r > T$ for an electric field with strength $\varepsilon > 0$ [Rat02]. Consequently, by following a temperature definition that is based on a no temperature-slip assumption at the boundary the identity is not recovered. In our view, both definitions of a reservoir temperature can be defended. Therefore, the issue about the existence or non-existence of the identity may be considered as undecided in this case.

As far as the Lyapunov sum rule introduced in Section III.B.2 is concerned, the situation is simpler. Replacing κ_b on the left hand side of Eq. (94) by the sum of Lyapunov exponents we may employ $dS = \varepsilon \langle v_x \rangle / T_r$ on the right hand side, which is the Joule heat that the particle gains during a free flight. Using furthermore $\sigma(\varepsilon) = \langle v \rangle / \varepsilon$ we obtain

$$\sigma(\varepsilon) = -\frac{T}{\varepsilon^2} \sum_{i=1}^4 \lambda_i(\varepsilon) \quad , \quad (95)$$

which, formally, is precisely the Lyapunov sum rule derived for the ideal Gaussian and Nosé-Hoover thermostats, cp. to Eqs. (33), (51). The only ambiguity is, again, whether T shall be identified with the temperature of the thermal reservoir or whether it shall be considered as a parameter in nonequilibrium by which the reservoir temperature T_r can be tuned accordingly, as discussed above. In any case, whether or not there holds an identity between phase space contraction and entropy production, here there exists a simple relation between the conductivity and the Lyapunov exponents of the system.

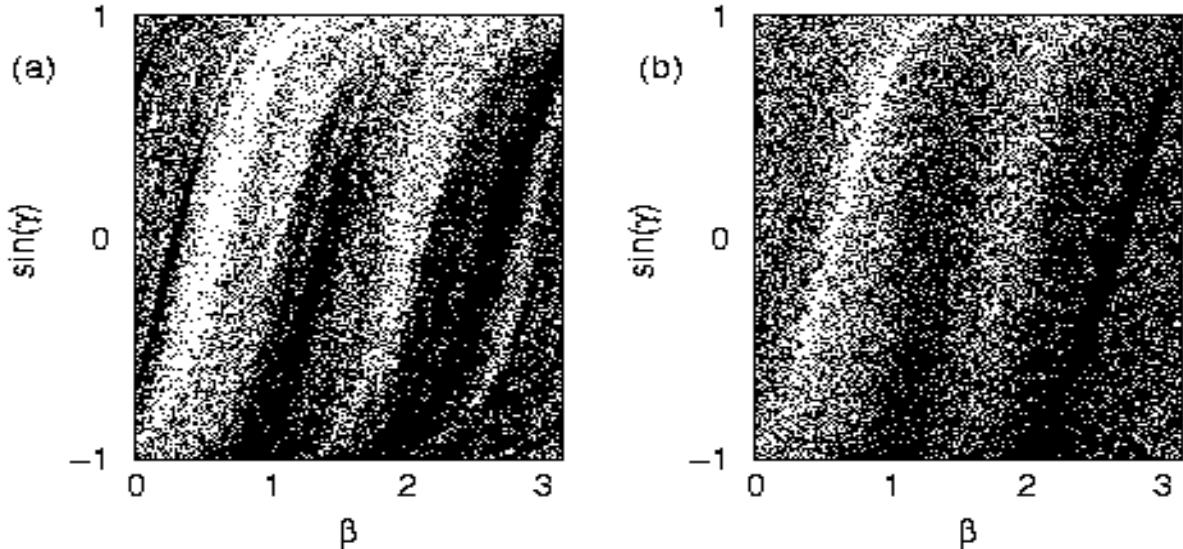


FIG. 16. Attractor for the periodic Lorentz gas driven by an electric field of strength $\varepsilon = 1$ which is parallel to the x -axis. The reservoir equilibrium temperature is $T = 0.5$, β and $\sin \gamma$ are defined in Fig. 4. In (a) the system is thermostated by deterministic scattering, see Eqs. (58), (89) and (90), in (b) it is thermostated by stochastic boundaries, see Eq. (89) and explanations. The results are from Refs. [Kla00b, Rat00b].

2. Attractors, bifurcation diagram and electrical conductivity

Fig. 16 shows two attractors for the driven periodic Lorentz gas thermostated at the boundaries, where all results presented for this thermostat are at $T = 0.5$. Part (a) displays simulation results for the deterministic boundaries Eqs.

(58), (89) and (90) adapted to the Lorentz gas geometry. Part (b) shows analogous results for stochastic boundaries, where the baker map Eq. (58) has been replaced by a random number generator. Both figures may be compared to the previous attractors Fig. 5 for the Gaussian thermostated Lorentz gas and Fig. 9 for Nosé-Hoover.

Clearly, the deterministic boundary solution exhibits a fractal-like folding, in analogy to the ones displayed for the Gaussian and for the Nosé-Hoover thermostat. In Fig. 16 (a) this structure just appears to be a bit more smoothed-out than for the Nosé-Hoover case. On the other hand, apart from a few non-uniformities on a coarse scale no fine structure is visible anymore for the attractor obtained from stochastic boundaries suggesting that Fig. 16 (b) does not represent a fractal set.

For deterministic boundaries the dimensionality of the attractor in the four-dimensional phase space was computed numerically by means of the field-dependent Kaplan-Yorke dimension $D_{KY}(\varepsilon)$ that was briefly mentioned in Section V.C [Rat02]. The results show that the dimensionality monotonously decreases from $D_{KY}(0) = 4$ to $D_{KY}(1) \simeq 3.7$ quantitatively confirming the fractality of the attractor in Fig. 16 (a). For Fig. 16 (b) respective computations are more subtle⁵⁴ and remain to be done. We emphasize that such computations would be very interesting, since according to our discussion in Section V.D it is not yet clear whether or not stochastically thermostated systems typically exhibit fractal attractors.

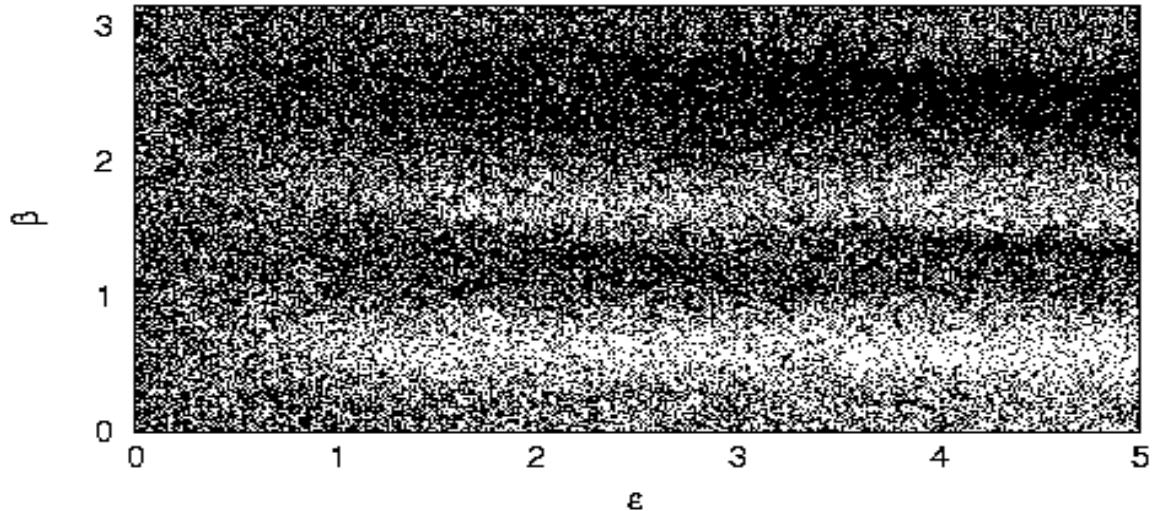


FIG. 17. Bifurcation diagram for the periodic Lorentz gas thermostated by deterministic scattering and driven by an electric field of strength ε which is parallel to the x -axis. The reservoir equilibrium temperature is $T = 0.5$, β is defined in Fig. 4. The figure is from Refs. [Kla00b,Rat00b].

The bifurcation diagram for the driven periodic Lorentz gas thermostated by deterministic boundaries is depicted in Fig. 17. Again, it should be compared to the previous counterparts Fig. 6 for the ideal Gaussian thermostat, Fig. 10 for the ideal Nosé-Hoover and Fig. 14 for the non-ideal Nosé-Hoover thermostat. Remarkably, in case of deterministic scattering there is no bifurcation scenario at all. That is, Fig. 17 neither shows a contraction of the attractor onto periodic orbits nor a breakdown of ergodicity for higher field strengths as it occurs for Gauss and Nosé-Hoover. Similar results have been obtained for other choices of projections in phase space as discussed in Ref. [Rat00b]. These results indicate that deterministic boundaries more strongly regularize the dynamics of the subsystem than Gauss and Nosé-Hoover. Furthermore, the different bifurcation diagrams clearly show that for simple systems such as the periodic Lorentz gas the deformations of the attractor under variation of the field strength intimately depend on the specific type of thermostating.

Fig. 18 finally contains the field-dependent electrical conductivity for the driven periodic Lorentz gas deterministically thermostated at the boundaries. In comparison to the conductivities corresponding to the ideal Gaussian, Nosé-Hoover and to the non-ideal Nosé-Hoover thermostats shown in Figs. 7, 11 and 13 (a), respectively, this curve looks rather smooth. As in the other cases, there is no indication of a regime of linear response in the numerically accessible

⁵⁴The Kaplan-Yorke dimension requires the computation of the full spectrum of Lyapunov exponents. Therefore, in case of stochastic boundaries one has to compute Lyapunov exponents for a stochastically perturbed dynamics; see also our discussion in Section V.D for respective difficulties.

regime of field strengths above $\varepsilon \geq 0.1$. On the other hand, again some wiggles on fine scales are visible suggesting that even for a bifurcation diagram such as Fig. 17 the corresponding conductivity might be, to some extent, an irregular function on fine scales. Note that the diffusion coefficient of the field-free periodic Lorentz gas thermostated by deterministic scattering may be different from the one for fully elastic scatterers and has not yet been computed. Hence, we do not know the prospective limiting value of $\sigma(\varepsilon)$ for $\varepsilon \rightarrow 0$ according to the Einstein formula Eq. (34).

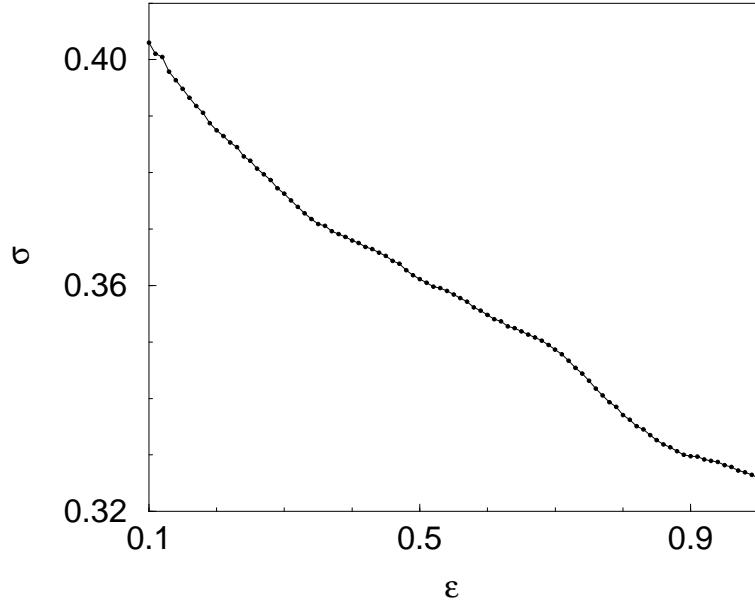


FIG. 18. Electrical conductivity $\sigma(\varepsilon)$ for the periodic Lorentz gas thermostated by deterministic scattering and driven by an electric field of strength ε which is parallel to the x -axis. The reservoir equilibrium temperature is $T = 0.5$. Each point has a numerical uncertainty that is less than the symbol size. The results are from Refs. [Kla00b,Rat00b].

3. Lyapunov exponents

By applying our deterministic boundary thermostat the kinetic energy is not kept constant at any instant of time, in analogy to Nosé-Hoover, but in contrast to the Gaussian thermostat. Consequently, this system is characterized by four Lyapunov exponents in the two-dimensional periodic Lorentz gas thermostated by deterministic scattering. Numerical computations of this spectrum of Lyapunov exponents turn out to be rather delicate due to the inelasticity at the collisions and require some more intricate adjustments compared to standard methods [Rat02].

For zero field numerical results corroborate that conjugate pairing holds with two zero, one negative and one positive Lyapunov exponent. However, in nonequilibrium there is no pairing of Lyapunov exponents anymore as shown in Fig. 19. This is in sharp contrast to the Lyapunov spectrum associated with bulk thermostats such as Gauss and Nosé-Hoover but appears to be typical for boundary thermostats, see our discussion in Section III.B.2. More precisely, one Lyapunov exponent is zero reflecting phase space conservation parallel to the flow. Two become negative and decrease monotonously in the field strength similar to power laws. Their functional forms remind of the non-zero exponents associated with the Gaussian thermostated driven Lorentz gas [Mor96a]. Indeed, as we have shown, for both thermostats there holds the Lyapunov sum rule, see Eqs. (33), (95). This equation, in turn, requires that the Lyapunov exponents are quadratic at least for small enough field strength.

The single positive Lyapunov exponent, on the other hand, displays a more intricate non-monotonic behavior under variation of the field strength. According to Pesin's theorem, see Section V.C, it must be equal to the Kolmogorov-Sinai entropy suggesting the following heuristic understanding of its functional form [Rat02]: For small field strength the particle attempts to move parallel to the field, hence the Kolmogorov-Sinai entropy decreases. However, by increasing the field strength the system starts to heat up in the bulk, consequently the Kolmogorov-Sinai entropy increases again. Such a behavior was not observed for the Gaussian thermostated Lorentz gas, where the Kolmogorov-Sinai entropy always decreases monotonically [Del95a,Det95], which is probably due to constraining the energy in the bulk.

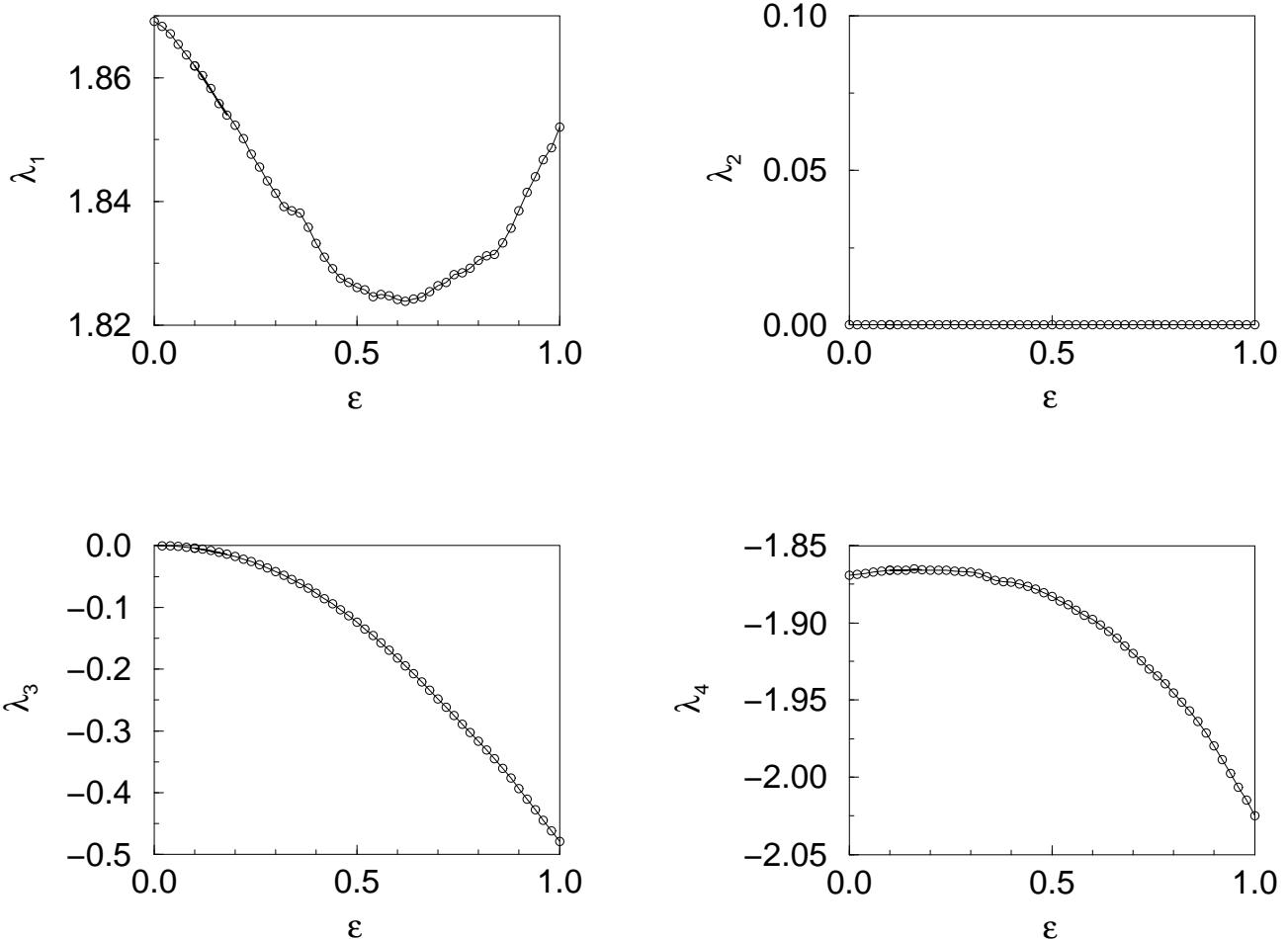


FIG. 19. The four Lyapunov exponents $\lambda_i(\varepsilon)$ for the periodic Lorentz gas thermostated by deterministic scattering and driven by an electric field of strength ε which is parallel to the x -axis. The reservoir equilibrium temperature is $T = 0.5$. The numerical uncertainty of each point is less than $5 \cdot 10^{-4}$. The results are from Ref. [Rat02].

E. Hard disk fluid under shear and heat flow

Up to now we have applied different schemes of thermostating to the driven periodic Lorentz gas only, which is a one-particle system that derives its statistical properties from the chaotic scattering of a moving point particle with a fixed hard disk. We deliberately chose a very simple model in order to focus on the impact that different thermostats have on this system. From this point of view, an important question is to which extent our findings concerning relations between chaos and transport still hold for many-particle systems that include interactions between different moving particles. Suitably amended periodic Lorentz gases of this type were already investigated in Refs. [Bar93, Bon97, Bon02]. Here we skip this intermediate step and immediately consider interacting many-particle systems for which hard disk fluids under nonequilibrium conditions are typical examples.

In a way, by looking at these systems we are back to the roots of thermostating: As explained in Chapters I to III, deterministic thermostats were originally designed as efficient tools within the framework of molecular dynamics computer simulations for driving large, interacting many-particle systems into well-defined NSS that are consistent with the laws of thermodynamics. That deterministically thermostated systems furthermore exhibit interesting chaos properties was only realized later on and subsequently motivated more specific studies of simple models such as the Nosé-Hoover oscillator and the thermostated driven Lorentz gas.

Here we move the other way around from simple to more complex systems. Particularly, we want to check whether for interacting many particles there is an identity between phase space contraction and entropy production, whether there are simple equations relating transport coefficients to Lyapunov exponents, and whether NSS are still characterized by the existence of fractal attractors.

As an example, we discuss a hard disk fluid under shear and heat flow. We start by briefly sketching various known

methods for modeling a shear flow. A well-known example are the *SLLOD* equations of motion representing the application of the conventional Gaussian thermostat for obtaining a sheared NSS. We then outline the construction of *Maxwell daemon boundaries* for modeling a hard disk fluid under shear. Finally, we discuss in more detail results for heat and shear flows generated according to thermostating by deterministic scattering, where we draw upon Refs. [Wag99,Wag00]. Interesting questions are whether these systems yield an identity between phase space contraction and thermodynamic entropy production and, correspondingly, whether there are Lyapunov sum rules for the respective transport coefficients. We furthermore summarize numerical results for the Lyapunov spectrum and for the Kolmogorov-Sinai entropy of this system.

1. Homogeneous and inhomogeneous modelings of shear and heat flows

Modeling and understanding shear and heat flows features as a prominent problem in nonequilibrium statistical mechanics. This is reminiscent by the existence of a huge literature on this subject. It is certainly not our goal to give a full account of all these works, in particular since many important aspects are nicely summarized in a number of reviews [All87,Eva90b,Hes96a,Hes96b,Hoo99,Mun00]. However, by mainly focusing on shearing we briefly describe at least some important approaches that have been pursued and to give a short account of investigations along the lines of connecting chaos and transport.

Probably the most naive way to shear a many-particle system is by using walls that move with certain velocities [Hes96a,Mun00]. Early attempts along these lines trace back to work by Hoover and Ashurst, see, e.g., Ref. [Hoo75] and also Refs. [Lie92,San92] for later investigations. Posch and Hoover used such *sliding boundaries* in combination with a Nosé-Hoover thermostat restricted to these boundaries [Pos89].

In contrast to this inhomogeneous driving from the boundaries, *Lees-Edwards* or *sliding brick* boundary conditions act homogeneously in the bulk of the system [All87,Eva90b,Hes96a,Hes96b,Hoo99,Mun00,Coh95]. The idea is to suitably displace copies of a unit cell of particles in space such that a linear shear profile is imposed onto the system. Lees-Edwards boundaries alone already yield a planar Couette flow for not too high shear rates. However, it turned out that this method could be improved by combining it with a Gaussian thermostat. In fact, the need to conveniently simulate sheared fluids and solids originally motivated the invention of the Gaussian scheme, cp. also to Section III.A [Hoo82,Eva83a]. Further refinements of the approach consisting of homogeneous shearing and Gaussian bulk thermostating eventually led to the formulation of the *SLLOD*⁵⁵ equations of motion [Eva90b,Eva90a,Sar92,Coh95,Hes96a,Mor89c,Sar98,Sea98,Mun00].

Curiously, by applying these shear flow algorithms to fluids consisting of hard spheres shear-induced microstructures were emerging in the simulations for high enough shear rates. That is, the particles were aligning themselves parallel to the direction of the flow in form of strings, or blocks (“plugs”). These orderings became known as the *string phase*, [Eva86,Eva90b,Mun00], respectively the *plug phase* [Loo90,Hes90,Hes96b,Hes97]. Partly it was argued that these phases represent artifacts of the homogeneous thermostating algorithms described above, since by construction these methods are adapted to the shear flow profile in a self-contained way [Eva86,Eva90b]. This led to the invention of more refined *profile unbiased* thermostating schemes (*PUT*) for which, partly, such structures were not observed anymore. Further refinements of PUT thermostats, on the other hand, reproduced these flow-induced positional orderings again [Loo90,Hes90]. To some extent, this problem reminds of our previous discussion starting from Chapter III, where we have shown that the application of different thermostats to the driven periodic Lorentz gas may yield different NSS. Here we appear to have a similar situation in the nonlinear regime of a sheared and thermostated many-particle system.

More recent work focused onto the connection between momentum transport and chaos properties of shear flows. It may not come as a surprise that, again, the SLLOD equations furnish an identity between phase space contraction and entropy production [Coh97]. Consequently, there is also a Lyapunov sum rule as already discussed in Section III.B.2 [Eva90a]. The most simple sheared systems allowing more detailed analyses are two-particle systems [Lad85] for which the existence of a shear viscosity could be proven [Bun96]. Morriss et al. [Mor87b,Mor89a,Mor89b,Pet94] extensively computed the complete spectra of Lyapunov exponents for such systems by showing that the phase space in these models contracts onto fractal attractors. Further numerical computations of Lyapunov spectra for sheared many-particle systems under application of conventional thermostating algorithms have been performed in Refs. [Pos89,Eva90a,Sea98,Sar92,Eva00]. Note that the existence of a conjugate pairing rule even in homogeneously

⁵⁵Concerning the origin of this name, which is not an acronym, see, e.g., Ref. [Mun00] and further references therein.

thermostated shear flows appears to be very delicate topic, as we have already outlined in Section III.B.2. We finally mention that even a multibaker map modeling a shear flow has been constructed and analyzed in Refs. [Tel01,Mat01]. Alternatively, Chernov and Lebowitz [Che95,Che97] proposed a many-particle shear flow model exhibiting a well-defined NSS without using a conventional thermostat. They considered a two-dimensional system of hard disks confined in a square box of length L with periodic boundary conditions along the x -axis, i.e., the left and right sides at $x = \pm L/2$ are identified. At the top and bottom sides of the box, $y = \pm L/2$, they introduced rigid walls where the disks are reflected according to certain scattering rules. The disks interact among themselves by impulsive hard collisions so that the bulk dynamics is purely conservative.

Shear is now introduced by imposing collision rules at the boundaries which turn the angle θ that the velocity vector of a particle moving towards the wall forms with the wall into an outgoing angle $\theta' := c\theta$, $0 < c < 1$. These “Maxwell daemon-like” boundaries mimic the impact of a shear force at the particle-wall interaction and enforce that particles move favorably parallel to the wall. Since energy is conserved by this operation the total energy of the particles is strictly kept constant thus reminding of the action of a Gaussian thermostat. Similar constraints have also been studied by other authors in different settings [Zha92,Ben01].

Chernov and Lebowitz used both time-reversible and irreversible formulations of such scattering rules. In both cases the resulting NSS of the hard disk-fluid were in full agreement with hydrodynamics. As a consequence of the specific scattering rules at the boundaries again the total phase space volume was not conserved. However, in this case the authors argued for an identity between phase space contraction and entropy production. Subsequent numerical studies of the dynamical instability of this system performed by other authors [Del97b] clearly showed that, as usual for boundary thermostats, the model exhibited no conjugate pairing rule. On the other hand, by using the full spectrum of Lyapunov exponents again evidence was provided for the existence of a fractal attractor in nonequilibrium. In further work the fluctuations of the entropy production of this model were investigated [Bon98a,Bon01].

As far as heat flows are concerned, general approaches to model the application of temperature gradients are summarized in Refs. [Hoo75,Hoo99,Eva90b,All87,Sar98,Kus02,Hoo03]. A mathematical analysis of Fourier’s law in some simple stochastic and Hamiltonian systems was provided in Refs. [Leb78,Eck99b,Eck99a,Mae03b]. Numerical implementations considered both stochastic [Ten82,Cic80] and deterministic boundaries, see, e.g., Refs. [Pos98,Hoo02b,Aok02,Kus02,Hoo03,Pos03]. Bulk thermostats were tested in Refs. [Hoo84,Hoo86]. In more recent work even a heat flow in a periodic Lorentz gas with rotating disks was studied [MM01,Lar03]. We remark that, apart from these works, there exists a vivid discussion about the validity of Fourier’s law in more simple models, partly also elaborating on the role of microscopic chaos, see Ref. [Lep03] and further references therein. However, here we will touch the heat flow case only very briefly by restricting ourselves to a specific many-particle system.

In the following we present results for a system consisting of a large number of hard disks that collide elastically with each other. This hard disk fluid is sheared and thermostated at the boundaries. The shear is modeled by moving walls, or sliding boundaries, imposing a local shear force onto the particles. In order to pump energy out of this system we use thermostating by deterministic scattering at the walls.

2. Shear and heat flows thermostated by deterministic scattering

We consider N hard disks that are confined between two flat walls as described above for the Maxwell daemon model. However, here we change the scattering rules at both walls according to Eqs. (58), (89) and (90), cp. to Fig. 15 and the respective discussion. Associating different temperatures T^u and T^d to the upper and the lower wall, respectively, enables us to study the case of a heat flow from a hot to a cold reservoir [Wag99].

For the simulations the length of the box was chosen to be $L = 28$ implying that the volume fraction occupied by $N = 100$ hard disks of radius $r = 1/2$ is $\rho = 0.1$. The temperature gradient was set according to $T^d = 1$ with $T^u = 1.5$ or $T^u = 2$. In both cases the temperature profile was found to be approximately linear, apart from boundary effects, and the kinetic energy of the particles was equipartitioned between the two degrees of freedom. As discussed in Section VII.D.1, assigning T^u and T^d as they appear in Eq. (89) to be the reservoir temperatures yields temperature jumps at the walls. This can be avoided by redefining the two reservoir temperatures according to smoothly extrapolating from the bulk to the boundaries under the assumption of equipartitioning of energy at the walls. In the following we take the latter point of view. Computing the thermal conductivity from simulations, the numerical results matched well to the predictions from Enskog’s kinetic theory [Ris96,Gas71]. This agreement improved by driving the system into the hydrodynamic limit. Hence, thermostating by deterministic scattering is able to generate a heat flow in a linear response regime that is in full agreement with hydrodynamics.

In a next step, the identity between phase space contraction and thermodynamic entropy production was checked for this situation. We do not go into too much detail at this point, see Ref. [Wag99] for an explicit discussion. However, there was good agreement between both quantities as obtained from computer simulations, which again improved

in the hydrodynamic limit, so in this case the identity was confirmed. We furthermore note that the ingoing and outgoing fluxes at the walls were approaching local thermodynamic equilibrium in the hydrodynamic limit. Starting from the same setup we now want to model the case of a shear flow. For this purpose we choose $T^u = T^d \equiv 1$. In addition, we wish that the upper and lower wall move with constant velocities d , respectively $-d$, opposite to each other. At a collision a hard disk must then experience the shear force

$$\mathcal{S}_d(v_x, v_y) = (v_x + d, v_y) \quad (96)$$

with d being positive (negative) at the upper (lower) wall. The main problem is to suitably combine \mathcal{S}_d with the action of the thermal reservoir at the wall. In Ref. [Wag99] three different options for linking \mathcal{S}_d with the thermostating rules Eqs. (58), (89) and (90) were explored. We first discuss

$$(v'_x, v'_y) = \begin{cases} \mathcal{S}_d \circ \mathcal{T}^{-1} \circ \mathcal{M} \circ \mathcal{T} \circ \mathcal{S}_d(v_x, v_y) & ; v_x \geq \pm d \\ \mathcal{S}_d \circ \mathcal{T}^{-1} \circ \mathcal{M}^{-1} \circ \mathcal{T} \circ \mathcal{S}_d(v_x, v_y) & ; v_x < \pm d \end{cases} \quad . \quad (97)$$

Requiring time-reversibility enforces us to apply \mathcal{S}_d symmetrically before and after the thermalization. Performing simulations for $d = 0.05$ and $d = 0.1$ the analysis proceeded along the same lines as for the heat flow: It was found that the system exhibited a linear shear profile for the average velocity parallel to the x -direction and a quadratic temperature profile between the walls, both as expected from hydrodynamics. Again, there were temperature jumps at the walls if the reservoir temperature T_r in nonequilibrium was identified with the equilibrium reservoir temperature T . A comparison of the viscosity computed from simulations with Enskog's theory [Gas71,Che95,Che97] yielded good agreement in the hydrodynamic limit, which is demonstrated in Table II. Thus, the combined mechanism of boundary thermostating and shear Eq. (97) generated a shear flow exhibiting a linear response regime in agreement with hydrodynamics.

We are now prepared to discuss the relation between phase space contraction and entropy production for this model. The average phase space contraction rate κ_b at the walls is defined in complete analogy to Eq. (92),

$$\kappa_b := \langle \ln \frac{|dv'_x dv'_y dx' dy'|}{|dv_x dv_y dx dy|} \rangle \quad . \quad (98)$$

Calculating the Jacobian determinant from the collision rules Eq. (97) yields

$$\begin{aligned} \kappa_b^{u/d} = & \frac{1}{2T^{u/d}} \langle v_x'^2 + v_y'^2 - v_x^2 - v_y^2 - \langle v'_x \rangle^2 + \langle v_x \rangle^2 \rangle \\ & + \frac{1}{2T^{u/d}} \langle \langle v'_x \rangle^2 - \langle v_x \rangle^2 - 2d(v'_x + v_x) \rangle \quad , \end{aligned} \quad (99)$$

where the angular brackets denote ensemble averages over moving particles. The temperatures $T^{u/d}$ are the reservoir equilibrium temperatures at the upper (lower) walls defined in Eq. (97).

Eq. (99) was already decomposed such that it can be compared to the thermodynamic entropy production of this system. For this purpose we consider again the Clausius form of entropy production in terms of the average heat transfer at the walls reading

$$dS = -\frac{1}{2T_r^{u/d}} \langle v_x'^2 + v_y'^2 - v_x^2 - v_y^2 - \langle v'_x \rangle^2 + \langle v_x \rangle^2 \rangle \quad . \quad (100)$$

	N=100	N=200	N=400	N=800
$d=0.05$	0.9616	0.9904	1.0081	1.0382
$d=0.1$	0.9702	1.001	1.0226	1.0232

TABLE II. Results for the fraction η_{exp}/η_{th} in a sheared fluid consisting of N hard disks. The shear viscosity η_{exp} was obtained from computer simulations, whereas η_{th} was calculated from Enskog's kinetic theory. The system is driven by boundaries moving with velocities $\pm d$ and thermostated by deterministic scattering at these walls, see Eq. (97). The values are from Ref. [Wag99].

Here $T_r^{u/d}$ stands for the reservoir temperature in nonequilibrium computed from the assumption that there is no temperature slip at the walls. Obviously, apart from the minus sign dS is formally identical to the first bracketed term in Eq. (99). As in Section VII.D.1, the issue is just whether one may identify the reservoir equilibrium temperature $T^{u/d}$ with the reservoir temperature $T_r^{u/d}$ under nonequilibrium conditions. Irrespective of this problem, the second term in Eq. (99) yields a contribution to the phase space contraction at the walls that has nothing to do with the thermodynamic entropy production of Eq. (100).

We may inquire whether this term has a possible physical interpretation. For the scattering rules Eq. (97) the average over in- and outgoing velocities parallel to the walls $u_w := (\langle v'_x \rangle + \langle v_x \rangle)/2$ is not necessarily identical to d . By assuming that it is at least some linear function of d the second line in Eq. (99) yields some correction of order d^2 . This contribution might be interpreted as a phase space contraction due to a friction parallel to the walls and may be thought of representing properties of a wall like roughness, or anisotropy of the wall scatterers.

In this respect our shear flow collision rules are very close again to the modifications that led to the non-ideal Gaussian and Nosé-Hoover thermostats discussed in Section VI.A and B. Note that for the latter types of thermostats the identity was destroyed due to what we called a *non-ideal coupling* between subsystem and reservoir. That is, we generalized the way subsystem and reservoir interact with each other by taking into account additional terms going beyond standard Gaussian and Nosé-Hoover frictional forces. Similarly, the above collision rules allow to incorporate further specificities into the microscopic subsystem-reservoir coupling. We conclude that such generalizations may lead to phase space contraction rates that are arbitrarily more complicated than the entropy production expected from thermodynamics.

That indeed the identity between phase space contraction and entropy production does not hold is quantitatively assessed by Table III. Here computer simulation results are presented for the fraction $-dS/\kappa_b$ of the entropy production dS , Eq. (100), divided by the average phase space contraction rate κ_b , Eq. (99). Clearly, the absolute values of both quantities are not the same, and the situation is getting even worse by approaching the hydrodynamic limit.

We remark that the entropy production in the bulk according to hydrodynamics [Che95,Che97] was also computed from the simulations. The result was again compared to the entropy flux across the walls in terms of the Clausius entropy yielding good agreement by approaching the hydrodynamic limit. In order to sort out the possibility that the non-identity specifically depends on the choice of the baker map in the collision rules Eqs. (97), the same simulations were carried out by replacing the baker with the standard map mentioned in Section VII.B, which was tuned such that its dynamics was approximately hyperbolic. However, instead of recovering the identity here the mismatch between phase space contraction and entropy production got even more profound [Wag99].

A more microscopic understanding concerning the origin of this inequality can be obtained by looking at the velocity distributions of the in- and outgoing particles at the walls. Fig. 20 shows that the two velocity components coming in from the bulk are nice Gaussian distributions at the wall. Indeed, the outgoing velocity distribution parallel to y is essentially indistinguishable from its ingoing counterpart. However, in sharp contrast to that the outgoing velocity distribution parallel to x exhibits a very irregular structure with some discontinuities. The explanation is that, according to the collision rules Eqs. (97), there will always be more out- than ingoing particles with $v_x \geq d$ at the upper wall (and with $v_x \leq d$ at the lower wall). Thus, due to normalization the two Gaussian halves in Fig. 20 (b) will never match to a full, nice Gaussian even in the hydrodynamic limit. Correspondingly, the associated in- and outgoing fluxes at the walls will never come close to a local thermodynamic equilibrium.

This motivates to check for the importance of local thermodynamic equilibrium at the walls concerning an identity between phase space contraction and entropy production. For this purpose a second set of time-reversible collision rules was constructed [Wag99] yielding local thermodynamic equilibrium at the walls in the hydrodynamic limit. However, the analytical result for the average phase space contraction rate already provided an equation that, again, was not identical to the entropy production Eq. (100), not even in the hydrodynamic limit. Computer simulations confirmed that, quantitatively, there is no identity either. Hence, these collision rules establish no identity even in case of local thermodynamic equilibrium at the walls.

	N=100	N=200	N=400	N=800
$d=0.05$	0.6761	0.5882	0.5023	0.4230
$d=0.1$	0.6457	0.5761	0.4934	0.4275

TABLE III. Computer simulation results for the fraction $-dS/\kappa_b$ in a sheared fluid consisting of N hard disks. The system is driven by boundaries moving with velocities $\pm d$ and thermostated by deterministic scattering at these walls, see Eq. (97). The entropy production dS was numerically computed from Eq. (100), the average phase space contraction rate κ_b from Eq. (99). The values are from Ref. [Wag99].

Eventually, a third set of collision rules was considered, again generating local thermodynamic equilibrium at the walls, however, by breaking time-reversal symmetry [Wag99]. In this case both the analytical expressions and the computer simulation results showed an identity between phase space contraction and entropy production in the hydrodynamic limit. Consequently, time-reversibility cannot be a necessary condition for an identity between phase space contraction and entropy production. This was already stated in Refs. [Che95,Che97,Nic98,Dae99] but seems to be at variance with conclusions drawn from the analysis of simple multibaker maps [Vol97,Bre98,Vol98,Tel00,Vol02]; see also Ref. [Mae03a] for a discussion of the relation between time-reversibility and entropy production on the basis of Gibbs states.

Typically, the existence or non-existence of the identity will have direct consequences for the validity of the Lyapunov sum rule as it was discussed in Sections III.B.2, IV.C.1, VI.A and VI.B. An exception to the rule was the driven periodic Lorentz gas thermostated by deterministic scattering where the identity was ambiguous, however, where in any case formally a Lyapunov sum rule was recovered, see Section VII.D.1. In other words, the identity is a sufficient condition for the validity of the Lyapunov sum rule but not necessary.

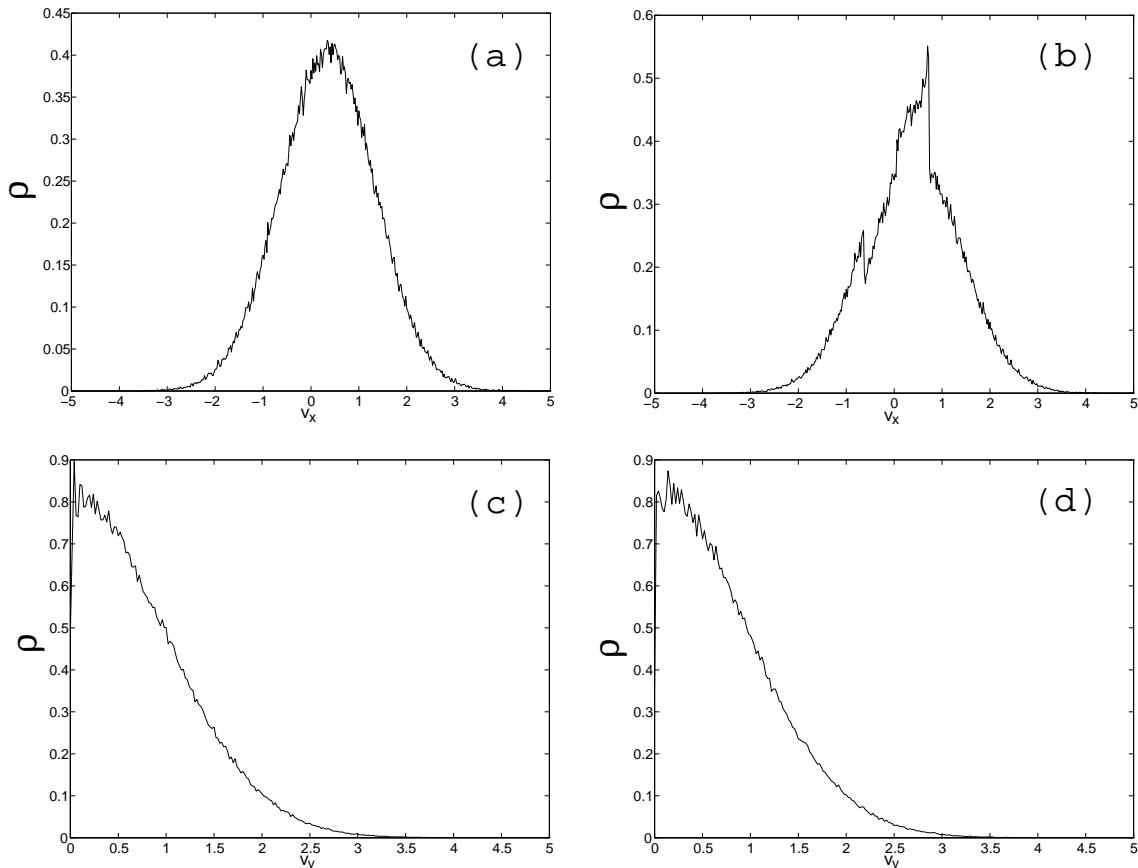


FIG. 20. Velocity distributions ρ at the walls for a sheared fluid consisting of N hard disks. The system is driven by boundaries moving with velocities $\pm d$ and thermostated by deterministic scattering at these walls, see Eq. (97). Shown are results for the velocity components v_x parallel and v_y perpendicular to the upper wall of the sheared system. (a) and (c) depict the distributions of velocities before the collisions with the wall, (b) and (d) the same after the collisions. The results are from Ref. [Wag99].

For the heat flow case outlined above the identity holds, hence there is a Lyapunov sum rule. On the other hand, a numerical computation of the Lyapunov spectrum shows [Wag00] that there is no conjugate pairing of Lyapunov exponents, as expected for a system that is thermostated at the boundaries. A computation of the Kaplan-Yorke dimension corroborates the existence of a fractal attractor. It might be interesting to construct collision rules that do not yield an identity for a heat flow, which should be possible along the lines as performed for the shear flow.

As far as the latter is concerned, for sake of comparison we first state the Lyapunov sum rule for the SLLOD equations. Here the identity holds and the shear viscosity η can be computed to [Eva90a,Coh95]

$$\eta(\gamma) = -\frac{T}{L^2\gamma^2} \sum_i \lambda_i(\gamma) , \quad (101)$$

where T is the temperature of the thermal reservoir, respectively the temperature pre-determined in the Gaussian thermostat, $\gamma := dv_x(y)/dy$ stands for the shear rate and L is again the system size.

For thermostating by deterministic scattering this relation may look rather different, depending on whether the identity holds. Let us consider the model for a boundary-driven shear flow Eqs. (97) explicitly discussed above for which there is no identity. By using the hydrodynamic relation $dS = L^2\gamma^2\eta/T_r$ and Eqs. (99), (100) one can nevertheless relate the viscosity of this model to the Lyapunov exponents arriving at

$$\eta(\gamma) = -\frac{T}{L^2\gamma^2} \left(\sum_i \lambda_i(\gamma) + O(d^2) \right) . \quad (102)$$

Here we have abbreviated the second line in Eq. (99) by the expression $O(d^2)$. Note that, in contrast to the non-ideal Gaussian and Nosé-Hoover thermostats of Sections VI.A and B, in this case we could at least establish an explicit relation between viscosity and Lyapunov exponents. Still, the viscosity is no simple function of Lyapunov exponents anymore thus providing a counterexample against a universality of the Lyapunov sum rule in thermostated interacting many-particle systems.

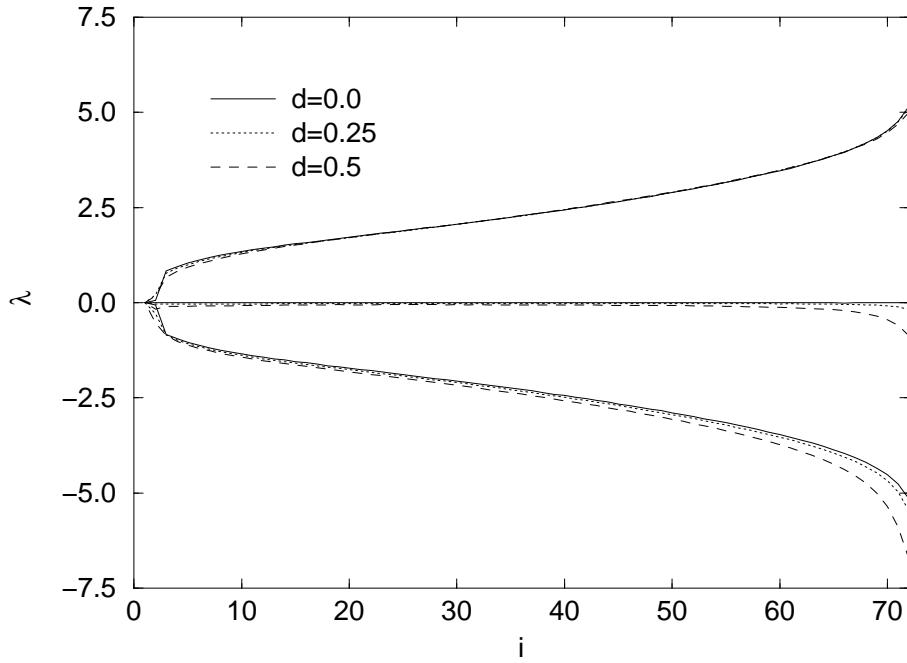


FIG. 21. Spectra of Lyapunov exponents λ for a sheared fluid consisting of 36 hard disks at a volume fraction of $\rho \simeq 0.47$. The system is driven by boundaries moving with velocities $\pm d$ and thermostated by deterministic scattering at these walls, see Eq. (97). Shown are results for three different driving forces as indicated in the figure. The lines in the middle represent the sums of conjugated pairs of Lyapunov exponents. The figure is from Ref. [Wag00].

Fig. 21 shows Lyapunov spectra for the shear flow generated from Eq. (97) in case of a system with 36 hard disks at a volume fraction of $\rho \simeq 0.47$, where the particles are in a quadratic box of length $L \simeq 7.746$. Depicted are results from simulations at three different shear forces d [Wag00]. The overall shape of these spectra is quite typical for sheared many-particle fluids [Mor89a,Mor89b,Pos89,Eva90a,Sar92,Del97a,Sea98]. However, note the asymmetry particularly between the largest positive and negative exponents. The sum of pairs of respectively ordered exponents is also included in the figure showing that, as in case of the heat flow, there is no conjugate pairing rule for the Lyapunov exponents.

Finally, we present results for the Kolmogorov-Sinai entropy of this system, which, according to Pesin's theorem, is identical to the sum of positive Lyapunov exponents. This quantity is plotted as a function of the shear rate γ for the same model parameters as in Fig. 21 above. The figure may be compared to the respective result for the driven periodic Lorentz gas thermostated by deterministic scattering, see λ_1 in Fig. 19. There is quite an analogy in that h_{KS} exhibits a global minimum by increasing the driving force. Curiously, for the non time-reversible collision rules

of the third model discussed above there is no such local minimum. Furthermore, the respective results for the heat flow of both models also do not exhibit a local minimum, see Ref. [Wag00] for further details. Computations of the Kaplan-Yorke dimension for the first and the third shear flow model yielded again evidence for the existence of fractal attractors. For a total of 144 phase space variables the associated loss of phase space dimensionality went up to about 6 at shear rates around $\gamma = 0.5$. Assessing the magnitude of the dimensionality loss became an active recent topic particularly by applying Gaussian and Nosé-Hoover thermostats restricted to boundary layers, after it was realized that the dimensionality loss may significantly exceed the number of constrained variables [Hoo02b,Aok02,Kus02,Pos03].

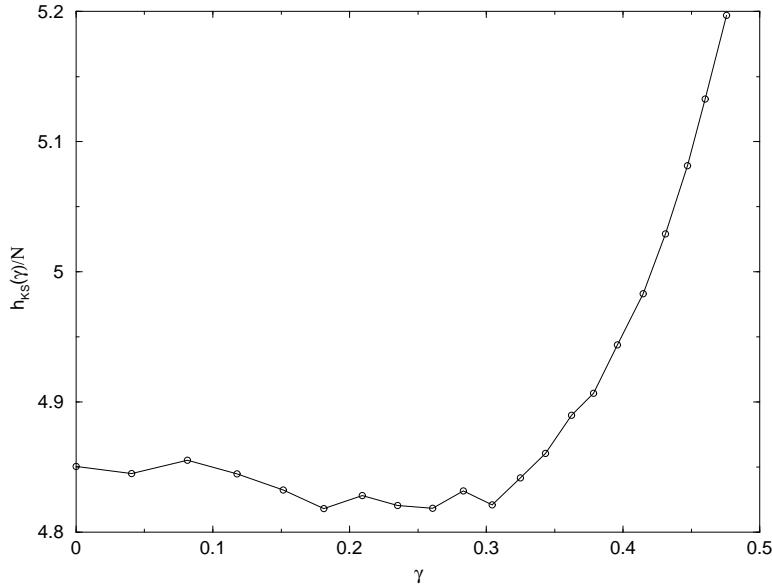


FIG. 22. The Kolmogorov-Sinai entropy h_{KS} per particle as a function of the shear rate γ for a fluid consisting of $N = 36$ hard disks at a volume fraction of $\rho \simeq 0.47$. The system is driven by boundaries moving with velocities $\pm d$ and thermostated by deterministic scattering at these walls, see Eq. (97). The figure is from Ref. [Wag00].

F. Summary

1. Modeling a stochastic thermal reservoir at the boundaries of a system is well-known in form of *stochastic boundary conditions*. The precise collision rules were briefly reviewed at the beginning of this chapter.
2. These stochastic collision rules can easily be made deterministic and time-reversible by using a deterministic map. The map should exhibit certain properties in order to enable a proper thermalization. The resulting deterministic and time-reversible boundary thermostat has been called *thermostating by deterministic scattering*.
3. Both types of boundary thermostats can be derived from first principles in three steps: Firstly, the precise functional forms of the equilibrium velocity distribution functions for arbitrarily many reservoir degrees of freedom are required, as they have been calculated earlier according to elementary equilibrium statistical mechanics. Secondly, one must define some coupling between subsystem and thermal reservoir. One then has to check whether the chosen coupling reproduces the correct velocity distribution functions. For arbitrary couplings this will not hold, typically. In this case one should enforce that the correct target velocity distributions are attained by suitably modifying the collision rules. For a nonequilibrium situation one needs to consider the limit of infinitely many reservoir degrees of freedom. Following this construction step by step sheds light again onto the origin of phase space contraction in thermostated systems, along similar lines as already elucidated previously.
4. As an example for the application of a deterministic boundary thermostat again the driven periodic Lorentz gas has been analyzed. Here the identity between phase space contraction and entropy production is ambiguous and depends on the definition of the temperature of the thermal reservoir. In any case, there is a Lyapunov sum rule for the electrical conductivity.

The attractor for the driven periodic Lorentz gas deterministically thermostated at the boundaries exhibits a fractal structure that is quite analogous to the previous ones resulting from ideal and non-ideal Gaussian and Nosé-Hoover thermostats. For stochastic boundaries this structure is not present anymore suggesting that the corresponding attractor is possibly not fractal. However, this conjecture remains to be verified quantitatively. In contrast to previous thermostated driven Lorentz gases the bifurcation diagram for the deterministic boundary thermostat is phase space covering for all values of the electric field strength. The electrical conductivity shows a nonlinear field dependence that is also different from the one obtained for other thermostats, being more smooth than in previous cases. Still, there are some irregularities on fine scales.

As is typical for boundary thermostated systems, there is no conjugate pairing rule of Lyapunov exponents for this model. The Kolmogorov-Sinai entropy related to the single positive Lyapunov exponents shows an interesting, non-monotonous behavior as a function of the field strength which has not been observed for bulk thermostats.

5. Finally, we have briefly summarized existing schemes that model shear flows for interacting many-particle systems, such as sliding boundaries, Less-Edwards ‘sliding brick’ boundary conditions, applying the Gaussian thermostat to shear in form of SLLOD equations of motion and refinements leading to PUT thermostats. For ideal Gaussian thermostats applied to modeling shear and heat flows there hold the usual relations between chaos and transport such as the identity between phase space contraction and entropy production and the Lyapunov sum rule. An alternative scheme was invented in form of Maxwell daemon boundaries and was argued to share the same properties. We also briefly outlined some conventional models of heat flows.

We then focused onto a hard disk fluid under shear and heat flow thermostated by deterministic scattering. For a heat flow this system exhibited linear response and yielded again an identity between phase space contraction and entropy production. For modeling a shear flow three different versions of a deterministic boundary thermostat were discussed. All of them generated a linear response regime. Two of them did not yield an identity and consequently no Lyapunov sum rule. One of them was not time reversible but reproduced the identity. Two of the shear flow models were analyzed in further detail showing that there was no conjugate pairing rule, as expected for thermostats acting at the boundaries. However, both models exhibited a fractal attractor. The latter properties are shared by the heat flow case. As in case of the respectively thermostated driven periodic Lorentz gas, the Kolmogorov-Sinai entropy displayed an interesting non-monotonous behavior as a function of the shear rate.

VIII. *ACTIVE BROWNIAN PARTICLES AND NOSÉ-HOOVER THERMOSTATS

In this chapter we return first to the Langevin equation reviewed in Section II.B. Langevin’s theory of Brownian motion presupposes that a Brownian particle is only *passively* driven by collisions from the surrounding particles. This input of energy is removed from the system by Stokes friction in the bulk leading to a balance between molecular stochastic forces and friction as formulated by the fluctuation-dissipation theorem.

Surprisingly, the Langevin equation can also be used to describe the motility of biological cells crawling on substrates, at least if the cell dynamics is sampled on large enough time scales. For experiments on moving cells such as granulocytes⁵⁶ and other types of crawling cells see Refs. [Fra90, Sto91, Sch93, Har94, Die03]; see also Refs. [Gru94, Rie00, Upa01] for related work where the cells move in more complex environments. In order to illustrate that cells may behave like Brownian walkers Fig. 23 depicts an experimentally measured trajectory of an isolated epithelial⁵⁷ cell moving on a substrate.

However, biological entities such as cells or bacteria may not really comply with the physical assumption of being particles that move only because of stochastic environmental forces. In order to sustain their motion such organisms rather need some external supply of ‘fuel’ that may be stored internally, and one may think of some metabolic activity converting the fuel into motion. This picture motivated to suitably amend conventional Langevin equations arriving at *active* Brownian particles that are able to take up energy from the environment, to store it onto internal degrees of freedom, and to convert it into kinetic energy [Sch98, Ebe99, Til99, Erd00]. Earlier models of active Brownian particles featured a response of these entities to environmental changes leading to pattern formation processes on a

⁵⁶These cells are attracted to sites of inflammation to destroy microorganisms and invaded cells.

⁵⁷An epithelial cell is one of the closely packed cells forming the epithelium, which is a thin layer of tissue that covers organs, glands, and other structures within the body.

macroscopic scale [Sch94,SG95]. Other recent work further generalizes active Brownian particles in order to describe confined systems with rotational excitations [Erd02,Ebe03].

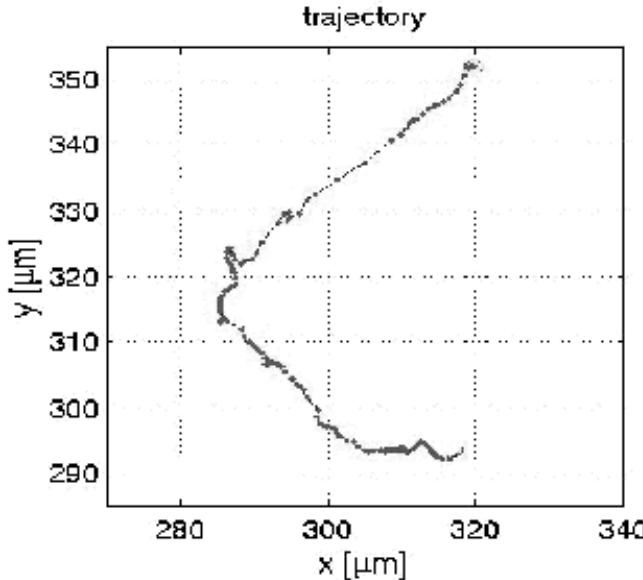


FIG. 23. Experimental results for the migration of an isolated renal epithelial MDCK-F (Madin-Darby canine kidney) cell on a substrate. The positions x and y were extracted from microscopic phase contrast images taken at time intervals of one minute and acquired for periods of two to four hours [Die03].

In the following we will argue that limiting cases of Langevin equations modeling active Brownian particles contain ingredients that trace back to the conventional Nosé-Hoover thermostat discussed in Chapter IV. This may not come too much as a surprise if one simply reinterprets the thermal reservoir associated with the Nosé-Hoover dynamics as the internal energy of a crawling cell. That is, instead of assuming the thermal reservoir to be ubiquitous and stationary one now deems it to be locally co-moving with the respective biological entity. Note that this merely amounts in suitably adapting the physical interpretation of the equations of motion, without requiring any reformulation of them. Similarly to deterministic thermostats, in our view such equations for cell motility may be considered as simple toy models that are proposed “top-to-bottom” on the basis of heuristic theoretical arguments rather than starting “bottom-up” from a detailed analysis of biological experiments. However, this approach may be useful for learning along which lines ordinary Langevin equations need to be modified in order to model the detailed dynamics of moving cells.

Here we review the formulation of active Brownian particles in terms of generalized Langevin equations. We show that a particularly simple limiting case of such equations exhibits formal analogies with the Nosé-Hoover thermostat. On the basis of the existing literature we then briefly summarize similarities and differences between active Brownian particles and Nosé-Hoover thermostats from a dynamical systems point of view.

In the second section we outline some essential features of the velocity distribution functions of active Brownian particles. We argue that the appearance of crater-like structures in their profile may be understood in connection with Nosé-Hoover thermostats. By employing the general functional forms of the equilibrium velocity distribution functions discussed in Section II.C we finally state some necessary conditions for the appearance of such crater-like structures.

A. Generalizing Langevin equations for modeling cell motility

The ansatz for modeling active Brownian particles which we review here starts from the generalized two-dimensional Langevin equation [Sch98,Ebe99,Til99,Erd00]

$$\begin{aligned} \dot{\mathbf{r}} &= \mathbf{v} \\ \dot{\mathbf{v}} &= -\alpha \mathbf{v} + \mathcal{F}(t) \quad , \end{aligned} \tag{103}$$

where \mathcal{F} is white noise, that is, a δ -correlated stochastic force of strength S with zero mean value,

$$\langle \mathcal{F}(0)\mathcal{F}(t) \rangle = S\delta(t) \quad . \quad (104)$$

The noise strength S can be straightforwardly associated with the friction coefficient α according to the fluctuation-dissipation theorem Eq. (2) and with the diffusion coefficient D by using the Einstein relation Eq. (3),

$$\frac{S}{2T} = \alpha = \frac{T}{D} \quad . \quad (105)$$

Let us now assume that there is a generalized friction coefficient α in form of

$$\alpha = \alpha_0 - de \quad . \quad (106)$$

Here α_0 holds for ordinary Stokes friction, the variable e denotes the internal energy of the moving entity, and the constant $d > 0$ yields the rate of conversion from internal into kinetic energy. e is in turn obtained from a suitable balance equation for which different choices have been discussed. A general ansatz, denoted in the following as *case 1*, reads [Sch98,Ebe99,Til99]

$$\dot{e} = \frac{1}{\mu}(q - e(c + dv^2)) \quad . \quad (107)$$

In this equation $q \geq 0$ describes a constant take-up of energy, which generally may be space-dependent, and c models some constant internal loss of energy. Note that d could be velocity-dependent, however, in Eq. (107) we stick to the most simple assumption that the prefactor of e is only quadratic in v . μ determines the rate of change of the internal energy e and thus plays a role similar to τ^2 in the Nosé-Hoover thermostat, see Eq. (44). In case of very fast feedback $\mu \rightarrow 0$ Eq. (107) boils down to the fixed point *case 2*,

$$e = \frac{q}{c + dv^2} \quad . \quad (108)$$

Combining this equation with Eq. (106) yields the velocity-dependent friction coefficient

$$\alpha = \alpha_0 \frac{v^2 - v_0^2}{\frac{q}{\alpha_0} + v^2 - v_0^2} \quad . \quad (109)$$

with $v_0^2 := q/\alpha_0 - c/d$. A special case of this type of friction is obtained by assuming $v^2 \ll v_0^2$, or alternatively $c/d \gg v^2$, in the denominator only leading to *case 3*

$$\alpha = \alpha_1 \frac{v^2 - v_0^2}{v_0^2} \quad . \quad (110)$$

with $\alpha_1 := -\alpha_0 + qd/c$. This equation is sometimes called the *Rayleigh-type model*, because a similar ansatz for a velocity-dependent friction coefficient has been introduced by Rayleigh in the context of the theory of sound [Erd00]. Eq. (110) looks strikingly similar to Eq. (44) defining the Nosé-Hoover thermostat. However, note that the former represents the explicit functional form for α , whereas the latter is a differential equation with a time-derivative for α on the left hand side.

Motivated by this formal similarity, one may ask to which extent models of active Brownian particles can exhibit dynamical systems properties as outlined in Chapter IV for the Nosé-Hoover thermostat. A fundamental difference between active Brownian particles and Nosé-Hoover thermostats is that the former have been introduced for modeling the energetic aspects of moving biological entities on a microscopic level, without knowing in advance about the velocity distributions generated by these models. In contrast to that, Nosé-Hoover thermostats have been constructed for generating, under suitable conditions, specifically canonical velocity distributions, see Section IV.B.1. A further difference already resulting from the Stokes friction coefficient is that the equations of motion for active Brownian particles are irreversible. But even more, according to ordinary Langevin dynamics these equations include noise, which is in contrast to the concept of Nosé-Hoover and other deterministic thermostats.

In order to bring active Brownian particles and deterministic thermostats closer together, thus making the three models introduced above more amenable to methods of dynamical systems theory, one may replace the white noise term by deterministic chaos, as we already briefly described in Section II.B. Another option is to generate deterministic chaos by choosing a suitable potential in configuration space such as the geometry of the periodic Lorentz gas, see the beginning of Section III.A. Yet we do not know anything about the velocity distributions for deterministic active Brownian particles and there is still the lack of time-reversibility. Hence, there is no reason why for these models

one should expect an identity between phase space contraction and entropy production to hold. Similarly, there is no reason why by default equipartitioning of energy should be fulfilled. Whether fractal attractors exist for this class of dissipative dynamical systems and whether Lyapunov sum rules and conjugate pairing rules hold, as they typically do for ideal Nosé-Hoover thermostats, are further interesting questions that have not been studied so far. However, we remark that for so-called canonical-dissipative systems containing active Brownian particles as a special case generalized Hamiltonian equations have been constructed that remind of the generalized Hamiltonian formalism developed for Gaussian and Nosé-Hoover thermostats outlined in Section IV.C.2 [Ebe00].

B. Crater-like velocity distributions

Let us now summarize what is known about the velocity distribution functions for the three different cases of active Brownian particles discussed above. In this framework we shall also discuss connections with the Nosé-Hoover thermostat.

In all cases, the most obvious solution for the velocity distribution is obtained at $e = \text{const}$. This is the Stokes limit of constant friction for which the velocity distribution is well-known to be purely canonical, see Section II.C.

For *case 1*, Eqs. (103), (106) and (107), not much appears to be known regarding general combinations of parameters in Eq. (107).

For the special *case 2* the situation is much better: Here the analytical solution for the velocity distribution function can be obtained from solving the corresponding Fokker-Planck equation and reads [Til99,Erd00]

$$\rho(v) = C \left(1 + \frac{dv^2}{c} \right)^{q/S} \exp\left(-\frac{\alpha_0}{S}v^2\right) , \quad (111)$$

where C is a normalization constant. Interestingly, as shown Fig. 24 this velocity distribution displays a transition from canonical to more microcanonical-like under variation of d or related parameters. Such *crater-like* velocity distributions exhibiting a dip at the place of the former maximum of the canonical distribution appear to be quite typical for active Brownian particles [Erd00,Sch01,Ebe01,Erd02,Ebe03].

Fig. 24 should be compared to our previous Fig. 8 displaying velocity distributions for the Nosé-Hoover thermostated driven periodic Lorentz gas. Apart from the asymmetry due to the external electric field the scenario is completely the same as in Fig. 24: By tuning the reservoir coupling parameter τ the Nosé-Hoover velocity distribution clearly shows a transition from canonical to microcanonical-like. The advantage of the Nosé-Hoover thermostat is that due to its construction the origin of these different functional forms is rather well-understood, as already outlined in Section IV.B.2: In the limiting case of $\tau \rightarrow 0$ the Nosé-Hoover thermostat generates a microcanonical velocity distribution, whereas in the limit of Stokes friction for $\tau \rightarrow \infty$ it yields a canonical one. Hence, there must be a transition between canonical and microcanonical for intermediate τ parameters. This transition is represented by a superposition of these two different velocity distributions.

For Fig. 24 and *case 2* a very similar explanation might thus be employed: The canonical velocity distribution is probably reminiscent of passive motion of the Brownian particles driven by the noise term in Eq. (103). The appearance of microcanonical-like features must then be due to the deterministic, velocity-dependent friction coefficient appearing in the equations of motion. This interplay may result in a transition from a canonical to a microcanonical(-like) distribution which is quite analogous to the one displayed by the Nosé-Hoover system. In contrast to Nosé-Hoover, however, for active Brownian particles this transition may rather reflect a change from noise-driven, passive motion to more active dynamics as determined by the deterministic, nonlinear part of the equations of motion.

On the other hand, we also have this formal analogy between the Nosé-Hoover equations of motion and at least *case 3* of active Brownian particles as noted in the previous section. If this link could be made more explicit one might argue that, irrespective of stochastic contributions in the equations governing active Brownian particles, there should as well be a Nosé-Hoover like transition in the velocity distributions which is purely generated by a tuning of the deterministic, velocity-dependent friction coefficient. This leads us to the conclusion that in case of active Brownian particles there may actually be two rather analogous transitions between canonical and microcanonical distributions, one that is of a purely deterministic origin and another one that is due to the interplay between deterministic and stochastic forces. To which extent the one or the other is exhibited by the dynamics may then depend on the specific choice of the control parameters.

We further remark at this point that an at first view analogous transition from unimodal to bimodal distributions has been reported for the stationary states of a nonlinear oscillator driven by Lévy noise [Che02,Che03]. However, the detailed dynamical origin of this transition appears to be very different from the two scenarios discussed above thus demonstrating that there may actually be a larger number of different dynamical mechanisms generating such bifurcations in the velocity distributions.

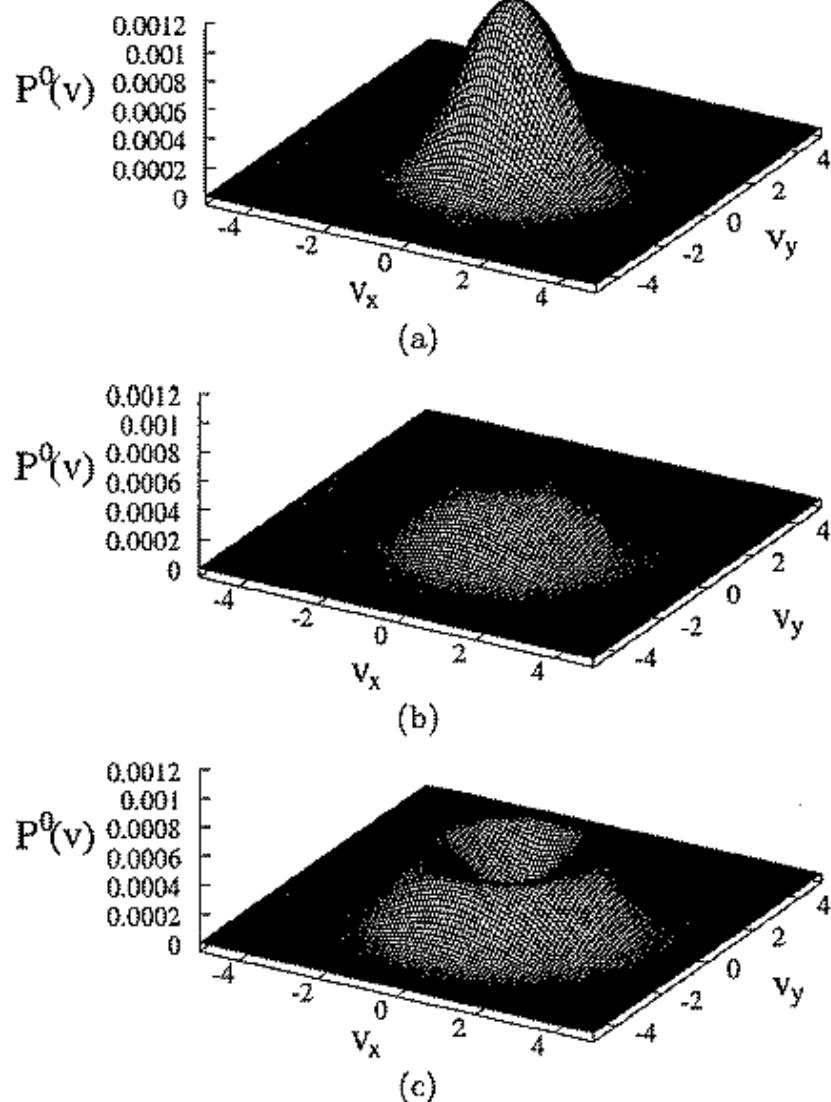


FIG. 24. Transition from canonical to *crater-like* velocity distributions in the model of active Brownian particles called *case 2*, see Eq. (108) in combination with Eqs. (103), (106). The figure displays the analytical solution $\rho(v) \equiv P^0(v)$ of Eq. (111). The parameters are $c = 1$, $q = 10$, $S = 4$, $\alpha_0 = 2$ and (a) $d = 0.07$, (b) $d = 0.2$, (c) $d = 0.7$. The figure is from Ref. [Erd00].

In order to undermine these arguments and before discussing the velocity distribution function of *case 3* in detail, let us analyze the transition between microcanonical and canonical distributions for the Nosé-Hoover thermostat more explicitly. Note that in the following we consider a purely deterministic equilibrium dynamics without any external field. We recall that the equation governing the velocity-dependent Nosé-Hoover friction coefficient α , Eq. (44), read

$$\dot{\alpha} = \frac{v^2 - 2T}{\tau^2 2T} . \quad (112)$$

In the limit of $\tau \rightarrow 0$ the Nosé-Hoover thermostat approaches the Gaussian one for which the kinetic energy is strictly kept constant at any time step. This suggests that the fluctuations of the friction coefficient α triggered in Eq. (112) by the remaining equations of motion should be getting smaller and smaller for larger times when the system is evolving into a steady state. Expanding Eq. (112) linearly in time yields

$$\alpha(t + \Delta t) = \frac{v^2 - 2T}{\tau^2 2T} \Delta t + \alpha(t) \quad (\tau \rightarrow 0, \Delta t \ll 1) . \quad (113)$$

As desired for thermalizing onto a steady steady this equation has a fixed point that in the limit of $\tau \rightarrow 0$ is associated

with the Gaussian thermostat constraint $v^2 = 2T$. However, if the first term on the right hand side of Eq. (113) were a non-zero constant the system cannot reach a steady state, since $\alpha(t) \rightarrow \pm\infty$. Hence, in this case $\alpha(t) = 0$ is the only steady state solution. For $\tau \ll 1$ small but finite $\alpha(t)$ fluctuates around zero corresponding to the time-dependence of v as induced by the other equations of motion. According to our above argument, for $\tau \ll 1$ these fluctuations may be suitably approximated by setting $\alpha(t) = 0$ on the right hand side of Eq. (113) thus recovering the functional form of the Rayleigh friction Eq. (110). Note that in the other extreme of $\tau \rightarrow \infty$ the friction coefficient α can be an arbitrary constant thus recovering Stokes friction, which in this equilibrium situation corresponds to zero velocity. We thus have a Hopf-like bifurcation scenario [Ott93] from $v = 0$ for $\tau \rightarrow \infty$ to a limit cycle behavior with $v = \text{const.}$ for $\tau \rightarrow 0$.

On the basis of this approximation, let us study what happens in the limit of small but finite $\tau \ll 1$ for the equilibrium velocity distribution function Eq. (42) of Nosé-Hoover reading

$$\rho(t, \mathbf{r}, \mathbf{v}, \alpha) = \text{const.} \exp \left[-\frac{v^2}{2T} - (\tau\alpha)^2 \right] . \quad (114)$$

The approximation Eq. (113) enables us to eliminate $\alpha(t)$ from the above equation yielding

$$\rho(v) = C \exp \left(-\frac{v^2}{2T} - \frac{(v^2 - 2T)^2(\Delta t)^2}{4\tau^2 T^2} \right) \quad (115)$$

$$= C \delta_\tau \left(\frac{(v^2 - 2T)}{2T} \right) \exp \left(-\frac{v^2}{2T} \right) \quad (\tau \ll 1, \Delta t \ll 1) \quad (116)$$

For the second line we have used the definition of the δ -function as a series of exponentials in τ [Rei65], where C is a normalization constant. We thus indeed arrive at the limiting case of a crater-like Nosé-Hoover velocity distribution composed of a canonical and a microcanonical contribution.

This solution may finally help to analyze the velocity distribution that was obtained for the active Brownian particle *case 3* [Erd00, Erd02],

$$\rho(v) = C \exp \left(\frac{\alpha_1}{S} v^2 - \frac{\alpha_2}{2S} v^4 \right) \quad (117)$$

with $\alpha_2 := \alpha_0 d/c$. The functional form matches nicely to Eq. (115) and there should be a respective decomposition into a canonical and into a microcanonical component in analogy to Eq. (116). However, there is the subtlety that Eq. (117) represents the solution for a stochastic system as is reminiscent by the strength S of the stochastic force. We therefore have to inquire whether this stochasticity is a crucial ingredient fundamentally distinguishing this distribution from the formally completely analogous but deterministic Nosé-Hoover solution Eq. (115).

Let us assume that in a suitable *case 3* system both the fluctuation-dissipation theorem and the Einstein relation are valid. According to Eq. (105) S is then a trivial function of the temperature T and the diffusion coefficient D . The temperature T may be defined by furthermore assuming equipartitioning of energy, $T = \langle v_0^2 \rangle / 2$, where $\langle v_0^2 \rangle$ is the average kinetic energy of the active Brownian particle. The diffusion coefficient D might be thought of being generated deterministically. We therefore argue that Eq. (117) also holds in a purely deterministic modeling of *case 3* thus establishing the connection to the Nosé-Hoover dynamics analyzed before. Under these conditions, *case 3* must exhibit the very same transition in the velocity distributions as Nosé-Hoover.

For sake of completeness we remark that in the limit of small velocities and by expanding the prefactor of the velocity distribution Eq. (111) of *case 2*, Eq. (117) of *case 3* is recovered again. Along these lines one may understand a transition such as the one depicted in Fig. 24 also on the basis of Nosé-Hoover dynamics.

To summarize, in all three cases of active Brownian particles discussed above there exists Stokes limit of constant friction yielding canonical velocity distributions irrespective of any stochastic contributions. We therefore conjecture that, in analogy to Nosé-Hoover dynamics, for *purely deterministic* active Brownian particles there exists a completely analogous transition from canonical to microcanonical velocity distributions under suitable parameter variation yielding intermediate crater-like velocity distributions. One choice for such a parameter variation should be varying μ in *case 1*, but other combinations of parameters, in analogy to varying τ in Nosé-Hoover dynamics, should be possible as well. For stochastic active Brownian particles defined in the framework of ordinary Langevin dynamics, *in addition* there should be a transition from a canonical velocity distribution function generated by the stochastic forcing to a microcanonical-like counterpart that, again, is due to a suitably tuned deterministic friction coefficient. This theoretical prediction still needs to be verified by computer simulations.

Finally, we briefly comment on two important necessary conditions limiting the range of existence of crater-like velocity distributions. For this purpose we remind again of the derivation of velocity distributions via projection

from a microcanonical one outlined in Section II.C. Let us assume that the velocity space of the moving particle has a dimension of $d \equiv d_s$, in order to be consistent with our previous notations. Let us furthermore assume that the d_s -dimensional velocity distribution of the moving particle is microcanonical as, for example, resulting from the application of a Gaussian thermostat, or in the limit of Nosé-Hoover dynamics for $\tau \rightarrow 0$. The central formula is then Eq. (19) telling us that *not* for any dimensionality d_s a one-dimensional projection $\rho(v_x) \equiv \rho(v_1)$ exhibits a crater-like minimum in its functional form.

More precisely, Fig. 2 shows that for $d_s \geq 3$ the particle's one-component equilibrium velocity distribution does not display a global minimum anymore. However, this eliminates any possibility for the generation of crater-like velocity distributions. That is, creating a transition from a projection of a microcanonical distribution to a canonical one (by noise, or by tuning τ in the Nosé-Hoover thermostat) for $d_s < 3$ cannot generate any non-monotonicities in intermediate distributions. In other words, for moving particles with more than two degrees of freedom there cannot be any transition between microcanonical and canonical one-component velocity distributions anymore featuring crater-like intermediate functional forms.

An analogous argument holds if the dimensionality d_r of an associated thermal reservoir can be changed as discussed, e.g., for thermostating by deterministic scattering in Section VII.C. For such a combination of subsystem and reservoir one can straightforwardly check [Kla], again by using Eq. (19) with $d \equiv d_s$, respectively with $d \equiv d_s + d_r$, that non-monotonous velocity distributions only appear if $d_s + d_r \geq 3$. These two bounds put therefore quite a window on the existence of crater-like velocity distributions.

Our discussion thus shows how deterministic thermostats such as Gauss, Nosé-Hoover and thermostating by deterministic scattering may help to understand the origin of velocity distributions in, at first view, seemingly quite different systems that may even be amenable to physical and biological experiments.

C. Summary

1. Results from experimental measurements on the motility of isolated cells moving on substrates can be understood, to some extent, by using conventional Langevin equations. Amended versions of such equations modeling the storage of internal energy of biological cells lead to the formulation of *active Brownian particles*.
2. We briefly reviewed three fundamental versions of active Brownian particles in which the friction coefficient of ordinary stochastic Langevin equations has been suitably generalized. The most simple model shared a striking formal similarity with the Nosé-Hoover dynamics discussed before. However, *per se* active Brownian particles and deterministic thermostats belong to the fundamentally different classes of stochastic, respectively deterministic dynamical systems.
3. We then discussed the origin of crater-like velocity distributions both for deterministic Nosé-Hoover dynamics and for stochastic active Brownian particles in thermal equilibrium. In case of Nosé-Hoover this transition is triggered by the tuning of the reservoir response time yielding a superposition between a microcanonical and a canonical distribution, as already mentioned in Section IV.B.2. Here we analyzed this scenario in more detail starting from the Nosé-Hoover equations of motion. Based on formal similarities of the underlying equations, we concluded that the same scenario must be present for active Brownian particles.

However, in addition the latter class of systems appears to feature a second mechanism leading to crater-like velocity distribution functions. In this case they result from a superposition between a stochastically generated canonical distribution and a microcanonical(-like) one related to the action of the deterministic friction coefficient.

Finally, we gave two necessary conditions concerning the involved number of degrees of freedom which must be fulfilled in order to generate transitions that are characterized by crater-like velocity distributions.

IX. CONCLUDING REMARKS

We begin this final chapter by briefly summarizing the main contents of this review. We then formulate our answer to the central question posed in this work by which we were inquiring about a general theory of NSS in thermostated dynamical systems starting from microscopic chaos. We furthermore list what we believe are important open questions and conclude with some acknowledgements.

A. A brief summary of this review

There are currently two fundamental approaches aiming at a general theory of NSS starting from microscopic chaos in the equations of motions of suitable model systems: One of them employs purely Hamiltonian dynamics supplemented by suitable (nonequilibrium) boundary conditions. The other one applies to nonequilibrium situations where a coupling to some kind of thermal reservoir is needed in order to sustain stationary solutions for statistical physical quantities. Typically, the latter approach renders the dynamical systems under consideration non-Hamiltonian due to a respective modeling of the thermal reservoirs. We have briefly outlined these two theories of chaotic NSS in our general introduction Chapter I. This review focused on the non-Hamiltonian approach to nonequilibrium transport, that is, on the construction and analysis of NSS in dissipative dynamical systems.

In Chapter II we motivated the use of thermal reservoirs both heuristically and by employing the Langevin equation, a well-known example for a stochastic modeling of thermostated dynamics. We sketched how to calculate the equilibrium velocity distribution functions for a subsystem coupled to a thermal reservoir and provided some general solutions. Finally, we introduced the periodic Lorentz gas, a standard model in the field of chaos and transport. In our review the model was connected to different thermal reservoirs. By applying simple nonequilibrium conditions we inquired about similarities and differences concerning chaos and transport properties in this model.

We started with two paradigmatic modelings of thermal reservoirs, which are known as the Gaussian and the Nosé-Hoover thermostat. These schemes go beyond ordinary Langevin dynamics in that the resulting equations of motion are still deterministic and time-reversible sharing fundamental features with Newtonian dynamics. The purpose of the Gaussian method is to transform the velocities of a subsystem onto microcanonical velocity distributions in thermal equilibrium. The Nosé-Hoover method was constructed to yield canonical velocity distributions. That is, for Gauss the total or kinetic energy is kept constant at any time step, whereas for Nosé-Hoover it is allowed to fluctuate canonically. If certain necessary conditions are fulfilled, applications of these schemes in nonequilibrium situations lead to well-defined NSS.

These two thermostats were introduced and analyzed in Chapters III and IV step by step. In order to motivate Nosé-Hoover dynamics we derived the (generalized) Liouville equation that is valid for dissipative dynamical systems. As a demonstration, we applied both the Gaussian and the Nosé-Hoover thermostat to the periodic Lorentz gas driven by an external electric field. We then discussed the resulting chaos and transport properties of these thermostated driven Lorentz gases. Additionally, we outlined generalized Hamiltonian and Lagrangian formulations for Gaussian and Nosé-Hoover equations of motion. This analysis was supplemented by reviewing more recent work concerning the construction of thermal reservoirs that generalize ordinary Nosé-Hoover dynamics.

Chapter V summarized our main conclusions concerning chaos and transport properties of NSS according to Gaussian and Nosé-Hoover theory. These preparations allowed us to start on the main question of our review, namely to which extent the chaos and transport properties discussed so far are universal for thermostated NSS altogether.

First answers to this fundamental question were provided in Chapter VI. Here we presented straightforward modifications of conventional Gaussian and Nosé-Hoover schemes leading to what we called non-ideal Gaussian and Nosé-Hoover thermostats. Again, we applied these mechanisms to the driven periodic Lorentz gas. It turned out that the non-ideal variants yield chaos and transport properties that are in many respects very different from conventional Gaussian and Nosé-Hoover dynamics.

All these thermal reservoirs acted directly upon the bulk of a subsystem to be thermostated. Chapter VII was therefore devoted to thermostats defined at the boundaries of a subsystem. A prominent example of this type of thermostats are stochastic boundary conditions. We showed that they can be reformulated in terms of deterministic and time-reversible collision rules making them comparable to Gaussian and Nosé-Hoover dynamics. This scheme, denoted as thermostating by deterministic scattering, was again applied to the driven periodic Lorentz gas. As in case of non-ideal thermostats, the chaos and transport properties obtained from this model were largely at variance with respective results of Gaussian and Nosé-Hoover dynamics. Asking for possible universalities of such properties in more complicated, interacting many-particle systems lead us to investigate a hard disk fluid under heat and shear. This system was also thermostated at the boundaries. Depending on the precise definition of the coupling between subsystem and reservoir, relations between chaos and transport known from ordinary Gaussian and Nosé-Hoover dynamics were either recovered or not.

Our review concluded with Chapter VIII by outlining further generalizations of ordinary Langevin dynamics. Here we discussed active Brownian particles providing abstract models for the motility of biological entities. We argued that there is a relationship between these models and conventional Nosé-Hoover thermostats. This is particularly reflected in the emergence of crater-like velocity distributions that are intermediate between canonical and microcanonical velocity distributions.

We emphasize that this review includes results that have not been published before. These are the construction and analysis of the non-ideal Gaussian thermostat, see Section VI.A, as well as Chapter VIII discussing the analogy

between active Brownian particles and Nosé-Hoover thermostats.

B. Do there exist universal chaos and transport properties of thermostated dynamical systems?

A central point of this review was to explore to which extent the description of NSS generated by conventional Gaussian and Nosé-Hoover dynamics is universal. In this endeavour Chapter V played a crucial role, where we summarized what we consider to be the most important links between chaos and transport resulting from Gaussian and Nosé-Hoover dynamics. On the basis of the analysis provided in Chapters VI to VIII we now briefly go through this list again and come to final conclusions.

1. **non-Hamiltonian dynamics for NSS:** In our view, this type of dynamics yields a rather natural description of NSS due to external forces. As we argued on many occasions, the non-Hamiltonian character of thermostated systems such as Langevin, Gaussian or Nosé-Hoover dynamics can be understood with respect to projecting out spurious reservoir degrees of freedom. From this point of view we do not see any reason to insist on a Hamiltonian modeling of NSS.
2. **phase space contraction and entropy production:** Conventional Gaussian and Nosé-Hoover thermostats display a default identity between these two quantities, which is at the heart of linking thermodynamics to dynamical systems theory in dissipative dynamical systems. However, it is not too difficult to construct counterexamples of deterministic and time-reversible thermal reservoirs generating well-defined NSS but not exhibiting this identity. We just mention non-ideal Gaussian and Nosé-Hoover thermostats and sheared hard-disk fluids thermostated by deterministic scattering. Care should therefore be taken exploring the second law of thermodynamics on the basis of this identity.
3. **transport coefficients and dynamical systems quantities:** Conventional Gaussian and Nosé-Hoover dynamics features the Lyapunov sum rule linking transport coefficients to Lyapunov exponents. However, the existence of such a simple functional relationship is intimately connected with the existence of the abovementioned identity. Hence, it is not surprising that this relation between chaos quantities and transport coefficients is not universal either. Non-ideal thermostats and thermostating by deterministic scattering yield again explicit counterexamples. We furthermore emphasize that there are broad classes of thermostated dynamical systems not exhibiting a conjugate pairing of Lyapunov exponents.
4. **fractal attractors characterizing NSS:** In all deterministically thermostated dynamical systems analyzed in this review the resulting attracting sets were characterized by fractal structures. This fractality is thus a very promising candidate for a universal property of NSS associated with deterministic and time-reversible thermal reservoirs. As it stands, it is also the only surviving one of the list of possibly universal characteristics discussed so far. However, note that the detailed topology of the attracting sets still intimately depends on the type of thermal reservoir applied. This is represented by the different types of bifurcation diagrams for the driven periodic Lorentz gas connected to different thermal reservoirs.
5. **nonlinear response in the thermostated driven periodic Lorentz gas:** Despite a mathematical proof for the existence of linear response in the Gaussian thermostated driven periodic Lorentz gas no clear signs of a regime of linear response could be detected in computer simulations for the Gaussian as well as for other thermostated Lorentz gases. Even worse, applying different thermostats yielded significantly different results for the field-dependent electrical conductivity of this model. We must therefore conclude that there is no equivalence of nonequilibrium ensembles for the thermostated driven periodic Lorentz gas in this regime of field strengths. In case of a thermostated hard disk fluid the situation appears to be better in that, at least, there is an equivalence of nonequilibrium ensembles as far as thermodynamic properties are concerned. However, we emphasize that on the level of chaos quantities there is no equivalence either.

We thus conclude that, from the point of view of nonequilibrium thermodynamics, the periodic Lorentz gas seems to be a rather delicate dynamical system. This appears to be due to the low dimensionality of the dynamics featuring a single moving point particle only. In this case statistical properties arise from the chaotic collisions of the particle with the fixed scatterers and contain intricate dynamical correlations in time and space. The different results for the field-dependent electrical conductivity presented in this review demonstrate the limits of standard thermodynamic descriptions applied to the thermostated model. However, in many other respects both the periodic Lorentz gas with and without external fields still exhibits “nice” thermodynamic behavior. And even the existence of irregularities in the field-dependent electrical conductivity should not be deemed “unphysical”: Interacting many-particle systems typically display thermodynamic behavior due

to their intrinsic statistical properties, whereas chaotically moving single particles may exhibit very intricate dynamical phenomena reflecting specific nonlinearities in their equations of motion. To us it appears that the periodic Lorentz gas, as well as multibaker maps, are right in-between these two large classes of high and low-dimensional, interacting and non-interacting many-particle systems. Such intermediate dynamics may thus display both ordinary thermodynamic behavior as well as specific chaotic dynamical properties. An adequate theoretical description thus needs to develop a well-balanced combination of both statistical and dynamical systems methods in order to adequately assess both the chaos and transport properties of this highly interesting type of dynamical systems.

C. Some important open questions

Here we only list a few basic problems that we consider worth to be studied in further research. More detailed open questions were already mentioned in the course of this review on various occasions.

1. **defining a nonequilibrium entropy:** This is of course a central question of nonequilibrium statistical mechanics altogether. From our point of view it is not enough to construct a theory of NSS starting from the ordinary Gibbs entropy. A proper definition of a nonequilibrium entropy should yield results that are compatible with standard nonequilibrium thermodynamics. In case of the driven Lorentz gas we think here of entropy production in terms of Clausius' entropy combined with Joule's heat. To us it appears that, apart from other problems, the Gibbs entropy may contain spurious contributions compared to a thermodynamic entropy production, since it samples the complete phase space which is at variance to an entropy production in terms of a heat transfer. This problem may be eliminated by using a revised definition of the Gibbs entropy based on a suitable coarse-graining. It might be interesting to apply such recent methods of coarse-grained entropies to our examples of thermostated dynamical systems not yielding an identity between phase space contraction and entropy production. One may hope that starting from such an amended Gibbs entropy ordinary thermodynamics can again be recovered even for our more general examples.
2. **fluctuation theorems:** We have said very little about this recent and very active research topic that concerns symmetry relations in the fluctuations of nonequilibrium entropy production. Apart from the fractality of attractors, fluctuation theorems currently feature as another important candidate for universal results characterizing NSS in dissipative dynamical systems. However, up to now fluctuation theorems have only been tested in thermostated dynamical systems furnishing an identity between phase space contraction and entropy production. It would thus be important to check for their existence in thermostated systems not featuring this identity, such as the ones described in our review. Interestingly, the existence of a certain class of fluctuation theorems is intimately linked to the validity of the chaotic hypothesis mentioned in the introduction. Hence, testing these fluctuation theorems one also studies, to some extent, the validity of the chaotic hypothesis. We furthermore suggest to look for fluctuation theorems in experiments on cell motility.
3. **existence of fractal attractors in stochastically perturbed dynamical systems:** As we have outlined on previous occasions, this important question is still not settled. In order to solve this problem one may study, for example, the driven periodic Lorentz gas or a hard disk fluid under shear supplemented by stochastic boundaries. It might then be elucidating to compare the respective results to the ones obtained from thermostated by deterministic scattering.
4. **analyzing NSS for generalized Nosé-Hoover thermostats and for active Brownian particles:** Following the philosophy of Nosé-Hoover there emerged a large collection of generalized deterministic and time-reversible thermostats for which it is still not clear to which extent they are functioning under nonequilibrium constraints. If they do, they may provide further access roads towards an analysis of chaos and transport properties of NSS going beyond ordinary Gaussian and Nosé-Hoover dynamics. The same reasoning applies to active Brownian particles that may be considered as another type of thermostated dynamical systems.
5. **quantum-mechanical formulations of thermal reservoirs:** In our review we did not say anything about extensions of classical deterministic and time-reversible thermostats towards the quantum regime. It seems that this field is currently evolving, see Refs. [Gri89,Kus93,Kus95,Men01,Kus02,Men03] and further references therein. Eventually, it might be interesting to study to which extent these approaches furnish links between chaos and transport being analogous to their classical counterparts.

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